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SELECT RESEARCH GROUP IN AIR POLLUTION METEOROLOGY,
SECOND ANNUAL PROGRESS REPORT
VOLUME II

THE PENNSYLVANIA STATE UNIVERSITY

PREPARED FOR
NATIONAL ENVIRONMENTAL RESEARCH CENTER

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IN AIR POLLUTION METEOROLOGY,
SECOND ANNUAL PROGRESS REPORT:
VOLUME II**

by

Select Research Group

Department of Meteorology and
Center for Air Environment Studies
The Pennsylvania State University
University Park, Pennsylvania 16802

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III BOUNDARY-LAYER MODELING

Task 1C

SECOND ANNUAL REPORT EPA-SRG

Task 1C - Boundary-Layer Modeling1. Summary of Progress

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Department of Aerospace Engineering

The task group is engaged in the development of model equations for the description of turbulence and diffusion in atmospheric boundary layers. Two major efforts are in progress. Under the direction of Dr. Lumley, a complete set of second-order turbulence model equations is being developed. Under the direction of Dr. Tennekes, simplified equations are used to study the development of convective boundary layers and the daily cycle of the mixing height. This latter work aims at improved boundary-layer parameterization schemes for use in with regional computer model of the Select Research Group.

The inversion-rise model developed by Tennekes during his sabbatical leave at the Royal Netherlands Meteorological Institute (1972-3) appeared to have the potential to produce short-term forecasts of temperature and mixing height. In cooperation with one of the Dutch meteorologists, this prospect has been explored. Very encouraging results have been obtained; they were presented at the AMS-WMO Symposium on Atmospheric Diffusion and Air Pollution (Santa Barbara, September 1974). A copy of the Santa Barbara paper is included in this report (Section 2, page).

This development suggested that a more detailed study of the convective boundary layer and of the turbulence dynamics near the inversion capping the boundary layer would be worthwhile. The mechanism of entrainment by which a boundary layer grows into the stable air aloft requires a more thorough analysis. It was decided to develop a computer program capable of reproducing the results obtained by Dr. J. C. Wyngaard of AFCRL; this program forms the foundation for further studies. The program has been developed by Otto Zeman; it is now ready for the planned work on the entrainment mechanism. Mr. Zeman's progress report is given in Section 3 (page).

In his attempts to formulate the equations necessary for his computer program, Mr. Zeman discovered that Rotta's simple model for the pressure-gradient velocity terms in the momentum-flux equations was inadequate, and that Lumley's current model for those terms was too cumbersome for his purposes. He developed an elegant and straightforward compromise; it is described in Section 4 (page).

In the system of equations developed by Dr. Lumley and Mr. Khajeh-Nouri, there is a large number of coefficients that have to be determined from experimental data. A search program for the optimum values of those coefficients in a plane isothermal turbulent wake was developed by Mr. Alan Huber. The results of this work are described in Mr. Huber's master's thesis (June 1974), of which copies have been sent to EPA. It is worth mentioning that Mr. Huber joined EPA at Research Triangle Park following his graduation.

Dr. Lumley and Mr. Khajeh-Nouri are continuing their development of a complete system of second-order equations for turbulent flows. Dr. Lumley has been on sabbatical leave in Europe during this past year; he has worked also on thermocline erosion in the ocean (a paper on that subject is in preparation), on the pressure-strain correlation, and on the turbulent flux of passive scalars in inhomogeneous flows. Much of this past year has been devoted to programming difficulties experienced with the simulation of a plane isothermal turbulent wake. Mr. Khajeh-Nouri's progress report is given in Section 5 (page), and Lumley's paper on the turbulent flux of passive scalar quantities is included here as Section 6 (page).

This concludes the summary of last year's progress in the two main areas of research. Other work included consultations with Dr. Anthes on boundary-layer parameterization, discussions with the EPA-staff on a visit to Research Triangle Park in December 1973, continuing discussions with Dr. Panofsky on coherence measurements and turbulent eddy structures, consultations on the design of the isokinetic aerosol sampling probe, and studies of the differences between Lagrangian and Eulerian statistics of turbulence. In this last area, which is crucial to the understanding of turbulent diffusion in the atmosphere, an interesting discovery was made concerning the shapes of the Lagrangian and Eulerian (sometimes called quasi-Lagrangian) correlation functions and spectra. A paper by Tennekes on this subject was accepted by the Journal of Fluid Mechanics; it is included here as Section 7 (page).

The research tasks of the Select Research Group encompass a great range of scales, ranging from the turbulent microstructure to synoptic scales of motion. Turbulence is generally analyzed with statistical methods, but mesoscale and large-scale atmospheric motions are handled with deterministic equations. The differences in approach make it difficult to maintain effective communications between those who study the larger scales and researchers concentrating on small-scale turbulence. In an attempt to provide a better understanding of these problems, Tennekes started a study of the similarities and differences between two-dimensional turbulence (which is a crude model for large-scale atmospheric flows) and three-dimensional turbulence. A first draft of a paper on this subject is included here as Section 8 (page).

2. SHORT-TERM FORECASTS OF TEMPERATURE AND MIXING HEIGHT ON SUNNY DAYS

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De Bilt, the Netherlands

1. INTRODUCTION

The inversion-rise models that have appeared in the literature recently (Betts 1973, Carson 1973, Tennekes 1973) contain prognostic equations for temperature and mixing height on sunny days without major advective changes. These equations appear to be useful for short-term forecasts of temperature, mixing height, and air-pollution index. This paper reports on studies made at the Royal Netherlands Meteorological Institute since the spring of 1973. In the first part of the paper, the inversion-rise model of Tennekes (1973) is used for forecasts pertaining to a fairly large number of days in 1971; in the second part, six representative forecasts are discussed in detail, and in the third part, progress in the determination of boundary conditions, initial conditions, and adjustable numerical coefficients is reported.

The equations developed by Tennekes (1973) do not account for advective changes, the presence of moisture, and large-scale subsidence. These effects can be incorporated if desired (Deardorff 1972, Betts 1973) but it was felt that a feasibility study such as this should concentrate on the validity of the basic model. The equations are

$$-(\overline{\theta w})_1 = \Delta \frac{dh}{dt} = c_1 (\overline{\theta w})_0 + c_2 \frac{T_0 u_*^3}{gh}, \quad (1)$$

$$h \frac{d\Delta}{dt} + \Delta \frac{dh}{dt} = \gamma h \frac{dh}{dt} - (\overline{\theta w})_0, \quad (2)$$

$$(\overline{\theta w})_0 - (\overline{\theta w})_1 = h \frac{d\theta}{dt}. \quad (3)$$

The symbols used here are defined as follows: h is the height of the inversion base, Δ is the temperature jump at the (idealized) inversion, θ is the potential temperature in the mixed layer (assumed to be independent of height), γ is the lapse rate of potential temperature above the inversion base, $(\overline{\theta w})_1$ is the turbulent kinematic flux of sensible heat at the top of the mixed layer (i stands for inversion base), $(\overline{\theta w})_0$ is the turbulent kinematic flux of sensible heat at the earth's surface, g/T_0 is a buoyancy parameter, and u_* is the surface friction velocity.

This system of equations can be solved if the initial conditions, the boundary conditions, and the constants c_1 and c_2 are specified. Preliminary studies (Tennekes 1973) showed that $c_1 = 0.2$ approximately. Also, the last term in (1) can be ignored if the wind speed is relatively low and the inversion height is greater than about 100 m. Therefore, we put $c_2 = 0$ for the first part of this study.

The initial conditions were taken from the temperature profile of the midnight radiosonde at De Bilt, the Netherlands. A minor adjustment was made for the observed minimum temperature at 1.5 m; this changed the initial temperature profile between 1.5 m and 50 m slightly, but it had no appreciable effect on the results.

The equations require that the surface heat flux be specified as a function of time of day and season. In the absence of direct observations it was decided to use climatological data on the annual cycle of the total amount of heat entering the atmosphere between sunrise and sunset on sunny days. These data, which are used for routine maximum-temperature forecasts by the Royal Netherlands Meteorological Institute, are readily available. The integrated heat flux obtained this way was converted into a curve representing the instantaneous heat flux by fitting a half a sine wave between sunrise and sunset such that the total area under the curve was equal to the heat-flux integral on which the operational maximum-temperature forecast is based. Later in this paper, we present measurements showing that these assumptions appear to be insufficiently accurate for the description of events during the early morning hours.

Calculations were performed for seventy-one selected days in 1971. The selection procedure discarded days with frontal passages, changes in air-mass origin, days with less than 20% sunshine, and days suspected to be influenced strongly by other advective effects. These trial forecasts were of an exploratory nature, and no attempt was made to account for subsidence, cloud cover, radiational cooling, latent-heat fluxes, and mechanical turbulence. The results of the calculations were compared with the observed temperature at 1.5 m in De Bilt, with the mixing height indicated by the noon radiosonde, and with the potential temperature in the mixed layer observed by the noon radiosonde.

2. STATISTICS

The observed maximum temperature at 1.5 m was compared to the forecast potential temperature in the mixed layer at sunset. The mean absolute value of the temperature difference, computed over 64 days (seven days had to be discarded because of computer program failure) was 1.5°C. The mean bias in the error was insignificant (0.3°C). These results are comparable in accuracy to those of the routine maximum-temperature forecast at the Royal Netherlands Meteorological Institute. This is not surprising, because the same heat-flux integral is involved. It should be noticed that the maximum temperature at 1.5 m is a surface-layer temperature, while the forecast temperature is a potential temperature in the bulk of the mixed layer. Also, the surface-layer temperature reaches its maximum earlier in the afternoon than the mixed-layer potential temperature. However, this inconsistency is ignored in the operational forecasts, too. In all likelihood, the temperature drop in the surface layer in the late afternoon approximately compensates the further heating of the bulk of the mixed layer during that period.

The noon (1200 GMT) radiosonde leaves De Bilt at approximately 12:30 p.m. local time. The observed potential temperature in the mixed layer at 12:30 p.m. was compared with the predicted temperature. The mean absolute value of the temperature difference, calculated over 59 days (some days had to be discarded because the radiosonde temperature profile did not show a well-defined adiabatic layer, and some others because of computer program failures) was 1.2°C. The mean bias in the error was negligible (0.3°C), showing that the method used does not introduce significant systematic deviations between forecasts and observations.

The height of the mixed layer at 12:30 p.m., as determined from the radiosonde temperature and humidity profiles, was compared to the forecast value. The mean absolute value of the height difference (calculated over 58 days) was 270 m; the mean bias in the difference was very small (11 m). The relatively poor accuracy may perhaps be ascribed in part to the poor vertical resolution of the radiosonde data, but it should also be kept in mind that the calculations did not account for subsidence and other advective effects. In order to obtain a preliminary assessment of the influence of advection, a subjective selection procedure was used to find a subset of days on which advective effects were small. This was done by comparing the temperature profile of the noon radiosonde with that of the preceding midnight radiosonde, and keeping all days in which the two soundings were nearly the same for the air above the mixed layer. A subset of sixteen days was found this way; the error statistics for this subset showed a slight improvement over those of the full set, except for a much improved mixed-layer height forecast at 12:30 p.m. (the mean absolute value of the error was 130 m for these sixteen days). This seems to indicate that the accuracy of forecasts of the height of the mixed layer can be improved by accounting for advective changes in the temperature profile of the air aloft. It is

worth noting that for this subset of sixteen days, the average percentage of sunshine was 75%, far greater than that of the complete set.

3. SIX REPRESENTATIVE FORECASTS

From the subset of sixteen days with small advective effects, six were chosen at random for a more detailed comparison between forecasts and observations. The predicted variation (with time) of the potential temperature in the mixed layer was compared with the temperature at 1.5 meter height as observed at De Bilt. The observed temperature thus is a surface-layer temperature. In convective conditions, the potential temperature at 1.5 m in the surface layer is higher than the potential temperature in the bulk of the mixed layer. Radiosonde data at De Bilt suggest that this difference is about 2°C around noon on sunny summer days, and about 1°C around noon on sunny winter days. This has to be taken into account when comparing the predicted curves with the observed ones.

The computed variation of the mixed-layer height was compared with the height indicated by the noon radiosonde and with the heights estimated by drawing an adiabat from the observed 1.5 m temperature each hour and determining its intersection with the temperature profile of the nearest radiosonde. This, of course, is an indirect estimate; however, no hourly data on the height of the mixed layer were available. The procedure followed here, incidentally, is identical to the one used to determine the late-afternoon height of the mixed layer from the observed maximum temperature at 1.5 m and the temperature profile of the noon radiosonde.

First example: forecast for April 15, 1971

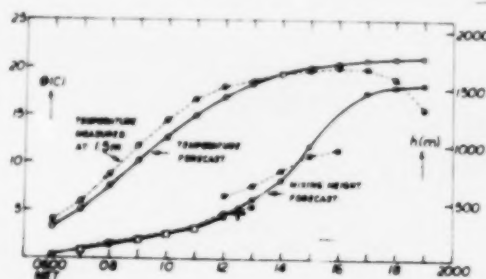


FIGURE 1: April 15, 1971

The temperature distribution at midnight on this day is characterized by a strong ground inversion, with a thickness of about 600 m. The stability of the layer of air between 600 and 1600 m, however, is small. This causes a rapid temperature rise in the morning hours and a very slow increase in the height of the mixed layer. Approximately 13:30 local time (MET), the mixed layer passes the 600 m level; subsequently, the height of the mixed layer increases - as expected - quite rapidly, while the temperature

increases very slowly. The observed maximum temperature at 1.5 m is 20.6°C; the maximum mixed-layer height estimated by drawing an adiabat from the observed maximum temperature is about 1350 m. The forecast height at the end of the day (sunset) is about 1600 m; it differs about 250 m from the estimated value.

Between 6:00 and 12:00 local time the difference between the observed temperature at 1.5 m and the calculated potential temperature in the mixed layer behaves approximately as expected; in the afternoon, however, the calculated temperature seems too high, even if the decreasing difference between surface-layer temperature and mixed-layer temperature is accounted for. In the late afternoon hours, the observed temperature decreases rapidly; this is (at least partially) a result of the way in which the surface layer reacts to the instantaneous heat flux (the surface heat flux changes sign about one hour before sunset).

The large cross in the figure is the height of the mixed layer as determined from the noon radiosonde data. This is the only time of the day on which a direct comparison between predictions and observations is possible. The mixed-layer height estimates based on late-afternoon surface-layer temperatures are not plotted in the figure, as they would suggest that the height of the mixed layer decreases after the maximum temperature is passed. Toward sunset, the surface-layer temperature decreases much faster than the temperature at higher levels (Figure 8).

Second example: forecast for April 26, 1971

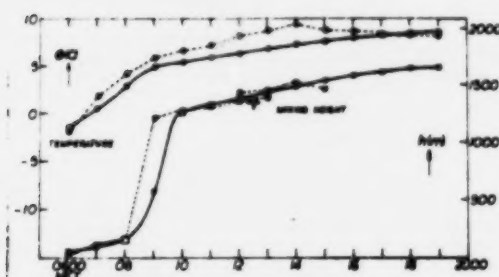


FIGURE 2: April 26, 1971

The temperature profile in the night preceding this day is characterized by a fairly thin ground inversion (up to 170 m), a nearly adiabatic region between 170 m and 1300 m, and a strong inversion - with a potential-temperature jump of 3°C - between 1300 and 1500 m. Both the calculations and the observations show that these initial conditions lead to behavior quite different from that observed on April 15.

The heating during the first two hours after sunrise causes a very rapid increase in temperature; this is characteristic for "burning off" a thin inversion layer, even if the heat flux is

relatively small. As soon as the near-adiabatic part of the temperature profile is reached, the mixed layer grows extremely rapidly; over a period of less than two hours the height of the mixed layer increases by about 1100 m. After 10:00 local time, the inversion height barely increases; this is caused by the constraints imposed by the inversion at 1300 m. Also, the temperature increases relatively slowly in this stage, because the heat flux is distributed over a layer of appreciable height. In early spring, the surface heat flux naturally is smaller than in the summer.

The difference between the observed temperature at 1.5 m and the forecast mixed-layer temperature behaves according to theoretical expectations. At sunrise, the two temperatures are nearly the same; around noon the surface layer is about 2°C hotter than the (potential) temperature in the bulk of the mixed layer. The two temperature curves intersect about an hour and a half before sunset (approximately when the actual surface heat flux changes sign).

This case clearly shows that the prediction method used here can also predict the time of day in which rapid changes occur. Such rapid changes are always associated with nearly-neutral layers in the air aloft.

Third example: forecast for July 11, 1971

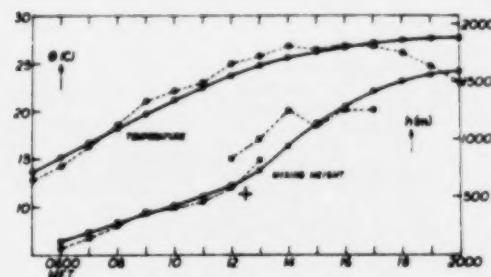


FIGURE 3: July 11, 1971

A ground-based inversion with a thickness of 600 m and a potential-temperature difference of 12°C marks the initial conditions for this day. In a very thick layer above this inversion, the lapse rate of potential temperature is about 3°C/km.

Even though this is midsummer, it still takes until about 13:00 p.m. local time before the nocturnal inversion is burned off. After that, the height of the mixed layer increases more rapidly, at least as long as the surface heat flux is still appreciable. The shapes of the curves are similar to those of April 15 (Figure 1). The predicted temperature appears to be on the low side; the difference between the temperature in the surface layer and the potential temperature in the mixed layer should be higher than indicated for a sunny summer day such as this.

Fourth example: forecast for September 5, 1971

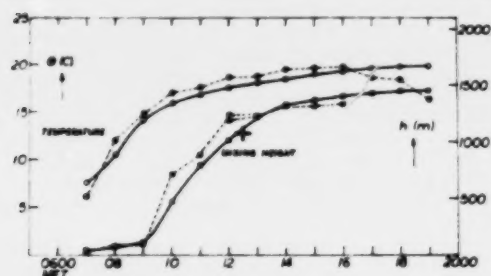


FIGURE 4: September 5, 1971

Just like April 26 (Figure 2), this is a case in which the initial conditions are characterized by a shallow ground inversion and a very stable layer between 1300 and 1600 m. The stability of the layer in between, however, is larger than it was on April 26. After the nocturnal surface-based inversion has been filled in (about 9:00 a.m. local time), the height of the mixed layer therefore does not increase quite as fast as it did on April 26. In cases of this kind, it is not hard to estimate the maximum height of the mixed layer, because the pre-existing inversion severely limits further growth in the afternoon.

The temperature cycle on this day sees a rapid increase during the filling of the nocturnal inversion and a slower increase in the following hours. The differences between predicted and observed temperatures appear to have reasonable values.

Fifth example: forecast for October 12, 1971

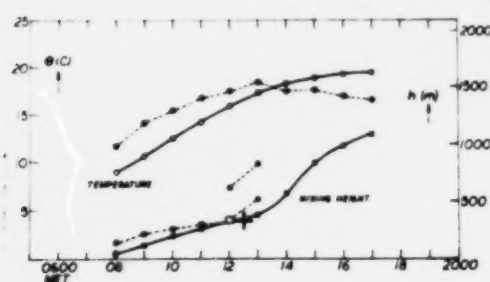


FIGURE 5: October 12, 1971

The midnight radiosonde data for this day show a ground inversion up to 350 m; above that level, the air is less stable. Approximately 13:00 local time, the ground inversion has disappeared; after that, the height of the mixed layer increases rapidly. The observed temperature reaches its maximum fairly early in the afternoon, so that the temperatures observed

after 13:00 local time could not be used to estimate the subsequent growth of the mixed layer. Nevertheless, the calculated maximum height of the mixed layer agrees well with the height estimated with the aid of the observed maximum temperature.

The differences between temperature forecast and observations are appreciable. The origin of this discrepancy is not clear. Possibly the prediction method is more sensitive to errors and inaccuracies when the total heat input is small.

Sixth example: forecast for October 24, 1971

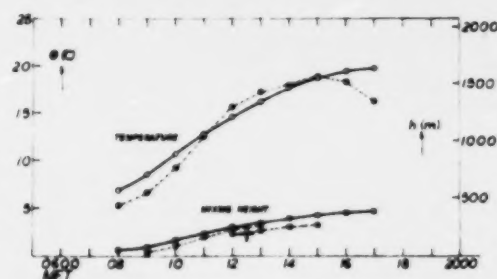


FIGURE 6: October 24, 1971

This is a day with an appreciable likelihood of serious air pollution. An inversion of 16°C, with a thickness of 400 m, characterizes the initial conditions. The heat supply is not sufficient to relieve this situation. Days such as this one are also marked by a large amplitude of the diurnal temperature cycle: at 8:00 local time, the temperature is 5°C, while the maximum temperature is 19°C. Such a large increase, notwithstanding the small heat supply, is made possible because the height of the mixed layer stays small.

4. FURTHER STUDIES

The instrumented 200-meter mast of the Royal Netherlands Meteorological Institute became operational in October 1972. It is located at Cabauw, 25 km SW of the Institute's headquarters in De Bilt. The mast has thermometers and anemometers at ten levels between 20 and 200 m; also, net radiation is measured at 2 m. The temperature measurements at the mast make it possible to determine the potential-temperature profile in the lowest 200 m; this provides accurate initial conditions. Also, there are several thermometer levels above the surface layer, so that the predicted potential temperature in the mixed layer can be compared with the potential temperatures observed at the higher levels on the mast. This procedure avoids the problems inherent to comparisons between observed surface-layer temperatures and predicted mixed-layer temperatures.

Radiation measurements taken at Cabauw during the first half of 1973 showed that a sine-wave approximation fits the daytime variation of the incoming net radiation very well on sunny days.

The curve, however, does not change sine at sunrise and sunset, but approximately one hour after sunrise and one hour before sunset (roughly when the sun is 10° above the horizon). We assumed that the upward flux of sensible heat at the surface is a constant fraction of the net radiation flux. After a number of trial forecasts, in which the constant of proportionality was varied over a wide range, it was determined that a factor of 0.43 gave the best overall fit between the forecasts and the observations.

The good vertical resolution of the temperature profile in the lowest 200 m allows an accurate determination of the initial values of Δ , θ , and h . One example is presented in Figure 7. The values h_0 , Δ_0 , and θ_0 at the beginning of the calculation are chosen in such a way that the initial inversion is represented in the best possible way. Figure 7 pertains to the initial conditions on May 27, 1973; moderately high wind speeds ($3-4 \text{ m sec}^{-1}$) maintained a low-level frictional inversion that night.

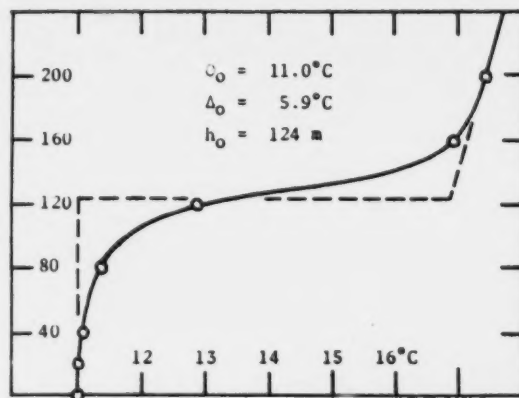


FIGURE 7: Initial Conditions for May 27, 1973

Further calculations were performed for 11 days in the period March-June 1973. These days were selected on basis of the following criteria: sunshine more than 65%, no rain or fog, and stationary large-scale weather conditions (in six cases), or clearly defined subsidence or advection effects (in five cases). For the five days with subsidence or advection, the initial conditions were adjusted to account for the trends associated with those effects. The adjustment procedure gave satisfactory results. Advective processes can be incorporated into the model without undue effort; however, the recognition of these processes remains a source for concern.

Various choices for the constant c_1 in (1) were tried. This constant determines the heat flux at the inversion base as a fraction of the surface heat flux in conditions with light winds. A satisfactory correlation between the predicted and observed mixing heights (the latter based on the noon radiosonde data) and between the predicted and observed potential temperatures in the mixed layer could be obtained only for $c_1 =$

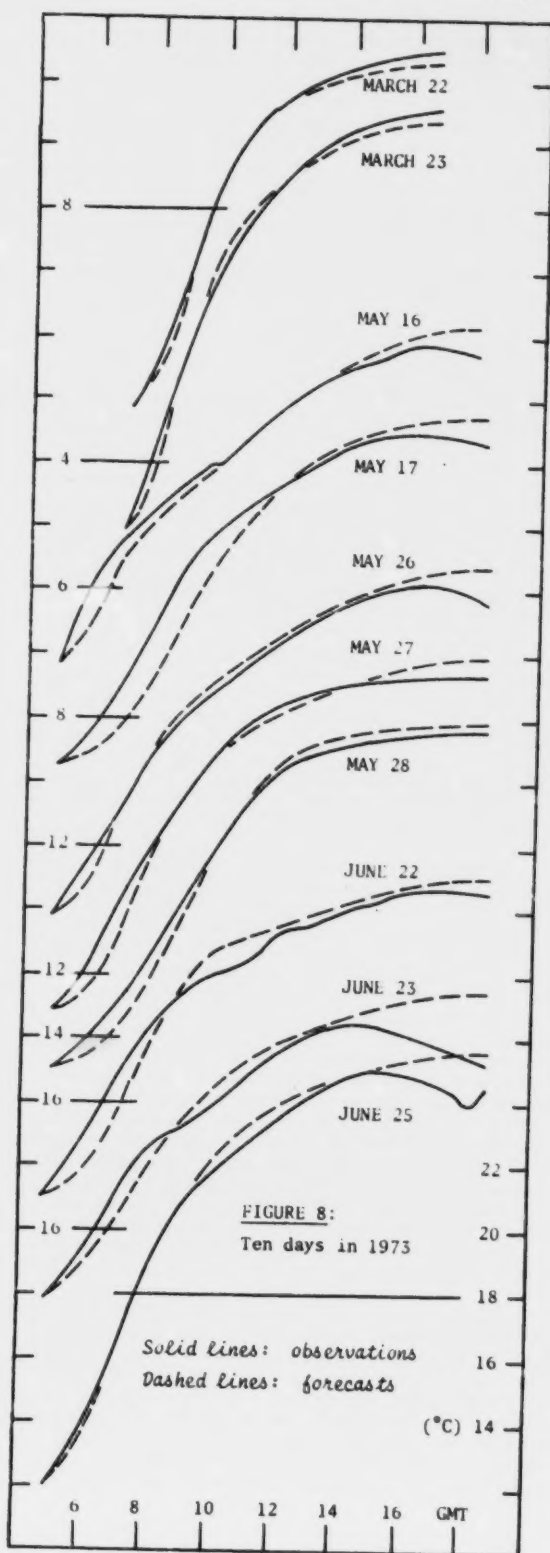
0.5. The use of $c_1 = 0.2$ (as in the first part of this paper) did not change the agreement between observed and predicted temperatures appreciably, but it caused the mixing height to be underestimated by some 10 to 50%, depending on initial conditions. Apparently, the use of $c_1 = 0.2$ is permissible only in the context of the heat-flux integral data employed in operational maximum-temperature forecasts. The source of this discrepancy has not yet been determined; we suspect that compensating errors are involved.

Because the early morning hours contribute relatively little to the growth of the mixed layer, the value $c_1 = 0.5$ should be representative of conditions during the middle of the day. This disagrees with the estimates made by Tennekes (1973) and Ball (1960), but it is in agreement with Carson's estimate. The latter (Carson 1973) is based on O'Neill data. We note that the frictional inversion-erosion term in (1) was neglected in all calculations reported here; it seems likely that the estimate $c_1 = 0.5$ will have to be revised downward if the frictional term (with a realistic value of c_2) is carried along in the calculations. The effect of the frictional term increases roughly as the cube of the wind speed; in a windy country such as Holland it may be necessary to include that term.

Comparisons between observed and predicted temperatures for ten days in 1973 are presented in Figure 8; they show that the agreement between forecasts and observations generally is quite good. For all cases, the forecast mixing height at 1200 GMT was within 200 m of the mixing height determined from the noon radiosonde; on six days, the difference was less than 100 m. For these calculations, we used $c_1 = 0.5$, $c_2 = 0$.

In the early morning hours, the forecasts provide a good fit to the data on days with low wind speeds. In the mornings of March 22 and 23, May 26, and June 25 the wind speed at 10 m was less than 3 m sec^{-1} ; for those days the predicted curve stays very close to the observed one. For the other six days significant deviations are found, which cannot be explained by possible errors in the initial conditions or in the heat-flux estimate. For all of these six days, the wind speed at 10 m was more than 3 m sec^{-1} ; for May 17 and May 28, it was about 6 m sec^{-1} . Clearly, the mixed layer was not in a state of free convection during the early hours of these days. Mechanical turbulence caused a larger downward heat flux at the inversion base, and a more rapid increase of temperature in the mixed layer. The effects of faster entrainment were visible in the shapes of the observed temperature profiles along the mast.

During the late afternoon the predicted temperature generally is higher than the measured one. This seems to suggest that the surface heat flux may decrease to zero somewhat earlier than the observed net radiation. In two cases, an alternative explanation can be given. On June 23 and June 25, wind direction changes were large; during the afternoons of these days, northerly winds advected cooler air toward the mast.



5. CONCLUSIONS

On days without major advective changes, the simple inversion-rise model used here appears to be able to describe the essential features of the daytime development of convective boundary layers quite well. The model requires a very limited input of data, and the computer calculations require only about a second per day. Operational use of a model such as this would seem to be feasible.

Several problems remain, however. In practice, relatively few days are characterized by stationary large-scale weather conditions; many more days throughout the year are affected by advective changes. Such changes can be incorporated into the model, but at this time it is not clear that this can be done successfully on an operational basis. This problem is particularly pronounced during the winter months, when the daily cycle of the surface heat flux plays only a minor role in the development of the boundary layer, so that a state of free convection does not occur all that often.

Another problem is that these forecasts cannot be made before the midnight radiosonde data are available. This limits the forecasting period to about 18 hours. In operational applications, however, forecasts of pollution-related parameters often have to be made for a 24-hour period; it is not clear whether the use of an estimated initial temperature profile would give sufficiently accurate results.

Acknowledgments

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3. ATMOSPHERIC TURBULENCE MODELING

Otto Zeman

Development of the Computer Program

As a prerequisite for detailed studies of the erosion of an inversion layer capping a convective boundary layer, a computer program was developed that simulates mean flow and turbulence in atmospheric boundary layers.

The program utilizes time-dependent ensemble-averaged equations for mean momentum, enthalpy, and turbulent fluxes. The DuFort-Frankel leapfrog method is used. This method has been successfully applied to a great number of fluid-dynamics problems and is well suited to the solution of non-linear differential equations in two independent variables (time and space). The solution proceeds from arbitrary initial conditions specified on the vertical axis between two boundaries at time $t=0$. As long as the initial values are reasonably well behaved, the time dependent solutions at time $t > 0$ converge to the desired steady-state solution, that is independent of the initial values. The rate of convergence is usually determined by the degree of turbulent diffusivity throughout the boundary layer.

Presently, the program is capable of predicting an entire neutral boundary layer or a convective layer capped with a rigid lid. The convective layer solution converges rapidly to its steady state. It requires only two CPU's on an IBM/370 to run a convective layer program at medium lid height to a Monin-Obukhov length ratio $(z/L) = -20$. The neutral layer solution converges relatively slowly, due to the large response time T , which is on the order of the inverse of the Coriolis parameter f ($T \sim 1/f$).

The program has a built-in flexibility to allow for incorporation of a variety of model equations, subsidence, moisture flux equations, etc.

At present the program is being prepared for study of the convective layer-inversion interface. Further, the program shall be put to use for the verification of the modeled terms in the turbulent flux equations.

Turbulence Model Equations, Boundary Values

In the case of a dry convective layer, a total of 15 equations have to be solved; in the case of a neutral layer, these reduce to nine equations. The upper boundary values are set at zero for all second moment turbulent quantities and for the mean velocity and temperature gradients. The upper boundary has to be placed high enough so as not to affect the solution below. The lower boundary is placed at a height where a neutral, constant stress layer is still existent. In other words, the ratio z/L has to be sufficiently small. Experimental constants and lower boundary values for all the quantities are in principle those used by Wyngaard (2).

The transport terms are modeled by gradient transport with an eddy viscosity proportional to the product of the kinetic energy and a turbulent time scale. The equation for the kinetic energy dissipation was adopted from Lumley (3).

Modeling of the Pressure Gradient-Velocity Term

The pressure gradient-velocity term (further PG-V) is represented in the equations of the present model by a single nonlinear return-to-isotropy term as proposed by Rotta:

$$\begin{aligned} A_{ij} &= \left\{ \frac{1}{\rho} \overline{u_j \frac{\partial p}{\partial x_i}} + \frac{1}{\rho} \overline{u_i \frac{\partial p}{\partial x_j}} \right\} - \frac{2}{3} (\overline{u_k p})_{,k} \delta_{ij} \\ &= - \frac{C}{T} (\overline{u_i u_j} - \frac{1}{3} \overline{q^2} \delta_{ij}) \end{aligned}$$

Although the model in this form can reproduce all the main features of the atmospheric boundary layer, it suffers from a serious shortcoming. The constant of proportionality of the return-to-isotropy terms has one value for the stress equation and another for the kinetic-energy component equations. It seems reasonable to require that the constants should be the same for all terms of the tensor A_{ij} . Furthermore, the model does not allow for differences in component energies in the cross-stream and vertical directions. It is known, however, from the experimental data that in the log-law region of neutral boundary layers, the cross-stream energy component is larger than the vertical one.

The fact that the single non-linear return-to-isotropy terms alone are not sufficient to represent the PG-V's has been long recognized by a number of researchers. The Poisson equation for the turbulent pressure fluctuation suggests that the mean shear be present in the PG-V model. Lumley (3) proposed terms which represent the effect of mean vorticity on the return-to-isotropy. Presently, there is a great number of PG-V models available. Most of the models suffer from either one of the following drawbacks:

- a) An excessive number of undetermined constants.
- b) Too many constraints imposed on the turbulent stress distribution.

In an attempt to avoid these pitfalls, we have developed two terms to be added to Rotta's original model, which include the effect of the mean strain rate and of the mean vorticity. Because in the neutral surface layer all transport terms become negligibly small, the equations for the turbulent second moments can be reduced to a set of three independent equations. With the known stress distribution, these equations allow for determination of the three unknown constants in the PG-V model. Details of the development of the new PG-V model are described in the next section ("Atmospheric Boundary

Layers and the Pressure Gradient-Velocity Correlation Model"). The new model allows for one numerical value of the constant C_1 of the return-to-isotropy terms in all equations and lends to the proposed model the desired universality.

Similar ideas will be applied to the heat flux equations.

Future Work

- 1) Incorporation of the proposed PG-V model in the turbulent boundary layer computer program.
- 2) Development of a quantitative model of the erosion of the inversion by a convective layer.
- 3) Study of details of the erosion layer using the computer program.
- 4) Study of large scale eddy transport in convective layers.
- 5) Computer simulation of the inversion rise.

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4. ATMOSPHERIC BOUNDARY LAYERS AND THE PRESSURE GRADIENT-VELOCITY CORRELATION MODEL

by

Otto Zeman

A pressure gradient-velocity (PG-V) model has been developed that gives realistic values of the turbulent stress components in the surface layer. The model consists of three terms: a nonlinear return-to-isotropy term (Rotta's model), a mean vorticity term, and a mean strain-rate term.

In the neutral surface layer, the turbulent stress equations can be reduced to three independent equations. For a given turbulent stress distribution, a unique set of three constants can be determined. The return-to-isotropy constant appears to be relatively insensitive to a variety of turbulent stress distributions.

Approach

If only Rotta's model is used, the turbulent stress equations in the neutral surface layer reduce to the following set:

$$[\overline{u^2}]: -2 \overline{uw} \frac{\partial u}{\partial z} - \frac{C_1}{T} (\overline{u^2} - \frac{1}{3} q^2) - \frac{2}{3} \epsilon = 0, \quad (1)$$

$$[\overline{v^2}]: - \frac{C_1}{T} (v^2 - \frac{1}{3} q^2) - \frac{2}{3} \epsilon = 0, \quad (2)$$

$$[\overline{w^2}]: - \frac{C_1}{T} (w^2 - \frac{1}{3} q^2) - \frac{2}{3} \epsilon = 0, \quad (3)$$

$$[\overline{uw}]: - \overline{w^2} \frac{\partial u}{\partial z} - \frac{C_1}{T} \overline{uw} = 0. \quad (4)$$

It can be shown that the set of equations (1) through (4) represent three independent equations. The turbulent equations in this form cannot reproduce the experimental data if the constant C_1 is to be the same for all four equations. Furthermore, $\overline{v^2} = \overline{w^2}$, so that the model does not allow for unequal values of the vertical and lateral component energies.

It is apparent that the equations in the surface layer can accommodate two additional terms with two undetermined constants. The additional terms were sought to possess the following properties:

- 1) To be of the same or the next higher order as compared to the original return-to-isotropy term and to be a function of the departure-from-isotropy stress tensor.
- 2) To reflect the effect of mean strain rate on the return to isotropy.
- 3) To reflect the effect of the mean vorticity on the return to isotropy. The turbulent stress equations contain explicitly certain terms in which the Coriolis parameter occurs. These terms influence the distribution of the normal stresses and the shear stress levels. It appears logical to represent the earth's rotation effect in the pressure gradient-velocity model.
- 4) The new terms have to have the correct tensorial properties, i.e., they have to be symmetric with zero trace.
- 5) There can be as many undetermined constants in the model as the number of independent equations allow, i.e., 3.

In view of the foregoing, we have selected additional terms as follows. Both have the proper symmetry and invariance properties.

- a) A tensor that contains accounts for the effects of the mean strain rate

$$A_{ij}^s \equiv b_{ik} S_{kj} + S_{ik} b_{kj} - \frac{2}{3} (Sb) \delta_{ij} ,$$

- b) A tensor representing the effects of the total vorticity

$$A_{ij}^v \equiv \Omega_{ik} b_{kj} - \Omega_{kj} b_{ik} .$$

Here, b_{ik} is the departure-from-isotropy tensor

$$b_{ik} \equiv \overline{u_i u_k} - \frac{1}{3} q^2 \delta_{ik} ,$$

S_{ik} is the mean strain rate tensor

$$S_{ik} \equiv \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} ,$$

$\Omega_{i\kappa}$ = vorticity tensor, defined by

$$\Omega_{i\kappa} = -\epsilon_{i\kappa\ell} \{ \overset{R}{\omega}_\ell + \overset{C}{\omega}_\ell \} ,$$

$\overset{R}{\omega}_\ell$ = relative vorticity vector, defined by

$$\overset{R}{\omega}_\ell = \{ \epsilon_{pr\ell} \frac{\partial U_r}{\partial x_p} \} \equiv \{ -\frac{\partial V}{\partial z}, \frac{\partial U}{\partial z}, 0 \} ,$$

$\overset{C}{\omega}_\ell$ = earth rotation vector, defined by

$$\overset{C}{\omega}_\ell = \{ 0, 2\omega \cos\phi, 2\omega \sin\phi \} .$$

The entire pressure gradient-velocity term is thus

$$A_{ij} \equiv -\frac{C_1}{T} (\overline{u_i u_j} - \frac{1}{3} q^2 \delta_{ij}) + \alpha A_{ij}^S + \gamma A_{ij}^V ,$$

where C_1 , α , γ are undetermined constants. Nondimensionalizing the turbulent stress equations in the surface layer by $u_*^3/\kappa z$, we obtain the following set of equations:

$$2(1-\alpha/3-\gamma) - (b_{11}/q^2)C_1/\beta - \frac{2}{3} = 0 , \quad (1^a)$$

$$4/3 \alpha - (b_{22}/q^2)C_1/\beta - \frac{2}{3} = 0 , \quad (2^a)$$

$$-2/3 \alpha + 2\gamma - (b_{33}/q^2)C_1/\beta - \frac{2}{3} = 0 , \quad (3^a)$$

$$-\frac{\overline{w^2}}{u_*^2} - \gamma \{ (b_{11}-b_{33})/q^2 \} \frac{q^2}{u_*^2} - \alpha (b_{22}/q^2) \frac{q^2}{u_*^2} + \frac{u_*^2}{q^2} C_1/\beta = 0 . \quad (4^a)$$

The equations (1^a) through (4^a) can be solved with C_1/β , α , and γ as unknowns. The constant β relates to the time scale used by Lumley ($\beta = T\epsilon/q^2$). For each set of ratios $\overline{u^2}/q^2$, $\overline{w^2}/q^2$, u_*^2/q^2 , there is a unique set of constants $\equiv C_1/\beta$, α , γ . The constants were calculated for six cases, representing experimental and arbitrary turbulent stress distributions. In all cases presented, the value of the constant C_1 is relatively insensitive to the stress distribution. Adopting Lumley's numerical value of β , which is 0.312, the value of C_1 is in the proximity of unity. The values of the constants α and γ seem reasonable; they are always positive and smaller than unity.

	#1	#2	#3	#4	#5	#6
$\overline{u^2}/q^2$	0.53	0.48	0.57	0.53	0.65	0.565
$\overline{v^2}/q^2$	0.25	0.38	0.28	0.33	0.23	0.34
$\overline{w^2}/q^2$	0.22	0.14	0.14	0.13	0.12	0.695
u_*^2/q^2	0.13	0.12	0.16	0.13	0.113	0.117
α	.291	.653	.393	.50	.23	.515
γ	.3705	.1225	.215	.152	.04	.1025
C_1/β	3.32	4.45	2.65	3.59	3.46	3.45

#1 An arbitrary stress tensor with $(\overline{v^2} - \overline{w^2})/q^2 \ll 1$, based on a modification of Wyngaard's data (reference 4)

#2 Cramer's data (reference 5)

#3 Mellor's data (reference 1)

#4 An arbitrary stress tensor with $b_{22} = 0$

#5 Comte-Bellot's data (reference 2)

#6 Hinze's data (reference 3)

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5: NUMERICAL MODELING OF TURBULENT FLOWS

B. Khajeh-Nouri

The first part of the year was spent in trying to find the reasons behind multiple roots for solutions to the turbulent shear equations. This multiplicity was first noticed when Mr. Huber's program for finding constants by trial and error kept giving different values. This program is based on finding the best set of constants to give the smallest mean square difference between the experimental and theoretical values. After writing a number of programs that could give themselves new and random starting positions in the space defined by the constants, it was possible to find a definite relationship among them. After this work the smallest (in terms of absolute value) values of the constants were used in the turbulent shear program.

During the first part of 1974, work was resumed on the equations of the turbulent shear program. The basic new assumption was that the amount of energy returned into a given direction must come from a direction rotated backward by the same amount that the flow has rotated. This means that the return to isotropy term in the turbulent shear equations is now expressed as

$$- \frac{(1 + 7II)}{T} \tilde{b}_{ij} q^2$$

where

$$T = \frac{cq^2}{\epsilon} \text{ is the time scale,}$$

ϵ is dissipation of turbulent energy,

$$q^2 = u^2 + v^2 + w^2 \text{ is the total turbulent kinetic energy,}$$

$$b_{ij} = \overline{u_i u_j} - q^2 \delta_{ij} / 3 \text{ is the rotated component, and}$$

II is the second invariant $b_{ij} b_{ji}$.

Here, $\tilde{b}_{ij}$ has its eigenvector rotated each by an amount depending on its original location. The total amount of the rotation cannot exceed 180° .

The characteristic time T was expressed as $t = \omega T$ where ω is a constant. The search for this constant and the use of the rotated b_{ij} 's was not very fruitful. However, it was an indication toward the next technique that was tried.

It was decided that the rotation cannot be expressed simply in terms of the rotation tensor Ω_{ij} , because the shear flow is a large distortion. Therefore, the whole expression for the expansion was redone using the whole $U_{i,j}$ term.

The expansion up to third order is

$$\begin{aligned}
& (1 + AII + 2E_1\Omega_{p\kappa}\Omega_{\kappa p})\{b_{ij} + v_1(b_{i\kappa}\Omega_{\kappa j} + b_{j\kappa}\Omega_{\kappa i}) \\
& + v_2(b_{ip}b_{pq}U_{j,q} + b_{jp}b_{pq}U_{i,q} - b_{ip}b_{jq}(U_{p,q} + U_{q,p})) \\
& + v_3(b_{ip}b_{pq}U_{q,p} + b_{jp}b_{pq}U_{q,i} - b_{ip}b_{jq}(U_{p,q} + U_{q,p})) \\
& + v_4(b_{ip}U_{p,q}U_{j,q} + b_{jp}U_{i,q}U_{p,q} - 2b_{pq}U_{p,i}U_{q,i}) \\
& + v_5(b_{ip}U_{p,q}U_{q,j} + b_{jp}U_{p,q}U_{q,i} - b_{pq}U_{i,p}U_{q,j} - b_{pq}U_{p,i}U_{j,q}) \\
& + v_6(b_{ip}U_{q,p}U_{q,j} + b_{jp}U_{q,p}U_{q,i} - 2b_{pq}U_{i,p}U_{j,q})\}
\end{aligned}$$

with the idea that everything was being rotated, every term is multiplied by the first term in parentheses,

$$(1 + AII + 2E_1\Omega_{p\kappa}\Omega_{\kappa p})$$

A, E_1 , V_1 , V_2 , V_3 , V_4 , V_5 and V_6 are constants. After some manipulation, the return-to-isotropy terms become:

$$\begin{aligned}
11 \text{ direction: } & b_{11} - b_{12}U'(V_1 - 2V_2b_{22} + 2V_3b_{11}) - 2U'^2(V_6b_{22} - V_4b_{11}) \\
22 \text{ direction: } & b_{22} + b_{12}U'(V_1 - 2V_2b_{22} + 2V_3b_{11}) + 2U'^2(V_6b_{22} - V_4b_{11}) \\
33 \text{ direction: } & b_{33} \\
12 \text{ direction: } & b_{12}[1 + (V_4 - V_5 + V_6)U'^2] + U'/2(b_{11} - b_{22})(V_1 - 2V_2b_{22} + 2V_3b_{11})
\end{aligned}$$

All of the terms are multiplied by

$$- \frac{q^2}{T} (1 + AII - E_1U'^2)$$

As before, programs were run to find the constants in the above expressions. The results were not satisfactory.

Another assumption was subsequently used to derive another set of expressions. This assumption claims that the expressions for the anisotropy for a lump of fluid is that seen a time T ago. Thus the non-rapid parts of the turbulent shear expressions should be something like

$$- \frac{(1+CIH)}{T} \{b_{ij} - aT(\frac{\partial b_{ij}}{\partial t} - \frac{\delta_{ij}}{3} \frac{\delta b_{PP}}{\delta t}) + \frac{a^2 T^2}{2} (\frac{\delta^2 b_{ij}}{\partial t^2} - \frac{\delta_{ij}}{3} \frac{\delta^2 b_{PP}}{\delta t^2})\} ,$$

where a is a constant taken to be of order one. The derivatives are intrinsic and depend on the deformation of the fluid system. Therefore the program for the deforming turbulent flow of Tucker and Reynolds changed also.

For a quasi-steady homogeneous flow, the derivatives become

$$\frac{\delta b_{ij}}{\delta t} = -U_{i,\kappa} b_{\kappa j} - U_{j,\kappa} b_{i\kappa} ,$$

$$\frac{\delta^2 b_{ij}}{\delta t^2} = U_{i,\kappa} U_{\kappa,\ell} b_{\ell j} + U_{j,\kappa} U_{\kappa,\ell} b_{i\ell} + 2U_{i,\kappa} U_{j,\ell} b_{\kappa\ell} .$$

The return-to-isotropy terms for deforming flow then become

$$A_{11} = -\frac{q^2}{T} (1+AD) \{b_{11} + \frac{2}{3} \gamma ST(2b_{11} + b_{33}) + \frac{2}{3} \gamma^2 S^2 T^2 (3b_{11} + b_{22})\} ,$$

$$A_{22} = -\frac{q^2}{T} (1+AD) \{b_{22} - \frac{2}{3} \gamma ST(b_{11} - b_{33}) + \frac{2}{3} \gamma^2 S^2 T^2 (b_{22})\} ,$$

$$A_{33} = -\frac{q^2}{T} (1+AD) \{b_{33} - \frac{2}{3} \gamma ST(2b_{33} + b_{11}) + \frac{2}{3} \gamma^2 S^2 T^2 (3b_{33} + b_{22})\} ,$$

$$D = b_{ij} b_{ji} \quad S^2 = \text{strain rate} \quad A = \text{constant}$$

γ = new constant to be determined.

The return to isotropy terms for turbulent shear flow become

$$A_{11} = -\frac{q^2}{T} (1+AD) \{b_{11} + \gamma TU' \frac{4}{3} b_{12} + \frac{2}{3} \gamma^2 T^2 U'^2 b_{22}\} ,$$

$$A_{22} = -\frac{q^2}{T} (1+AD) \{b_{22} - \frac{2}{3} \gamma TU' b_{12} - \frac{1}{3} \gamma^2 T^2 U'^2 b_{22}\} ,$$

$$A_{33} = -\frac{q^2}{T} (1+AD) \{b_{33} - \frac{2}{3} \gamma TU' b_{12} - \frac{1}{3} \gamma^2 T^2 U'^2 b_{22}\} ,$$

$$A_{12} = -\frac{q^2}{T} (1+AD) \{b_{12} + \gamma TU' b_{22}\} .$$

Because of these changes, γ and the time constant c in the expression, $T = cq^2/\epsilon$, become the only constants to be searched for. When these changes were put into the respective programs, the deforming turbulent flow would not work for any value of γ or c . However, the shear flow did work but for strange values (not near one) of γ . Realizing that the shear program did work gave a clue as to the direction one should take in trying to solve the problem.

This was to realize that q^2 is transported like a scalar in a boundary layer. To represent this we must deal with $u^i u_j$ and not $u_i u_j$. Hence, we should have

$$- \frac{(1+cII)}{T} [b_j^i - aT \frac{\delta b_j^i}{\delta t} + \frac{a^2 T^2}{2} \frac{\delta^2 b_j^i}{\delta t^2}] .$$

The contravariant indices do not matter to us as we are in Cartesian i coordinates but the signs of the terms do. Thus in this case since $U_{,j}$ and b_j^i are in the same principal axes, both derivatives

$$\frac{\delta b_j^i}{\delta t} \quad \text{and} \quad \frac{\delta^2 b_j^i}{\delta t^2}$$

are identically equal to zero.

This means all of the equations in the deforming turbulent flow stay exactly the same. The turbulent shear terms now become

$$A_{11} = - \frac{q^2}{T} (1+AD) [b_{11} + \gamma T U' b_{12}] ,$$

$$A_{22} = - \frac{q^2}{T} (1+AD) [b_{22} - \gamma T U' b_{12}] ,$$

$$A_{33} = - \frac{q^2}{T} (1+AD) b_{33} ,$$

$$A_{12} = - \frac{q^2}{T} (1+AD) [b_{12} - \frac{\gamma T}{2} U' (b_{11} - b_{22}) - \frac{\gamma^2 T^2 U'^2}{2} b_{12}] .$$

The value of γ was searched for in the seeker program and was found to be + .25. This produced very good results in all of the component energies but the uv graphs were 1/3 less than the experimental values.

The work is now at this point. Obviously new values for the $\overline{uv}$ term must be found from modifications of the theory. This is now in progress.

6. MODELING TURBULENT FLUX OF PASSIVE SCALAR
QUANTITIES IN INHOMOGENEOUS FLOWS*

by

John L. Lumley**

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Summary

It is suggested that, in an inhomogeneous turbulent flow, the flux of a passive scalar admixture should be modeled to first order by a linear combination of gradient transport and convective transport, where the convective transport coefficient is proportional to the *gradient* of the (gradient)-transport coefficient. A simple model is presented which allows determination of the coefficient of proportionality.

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It is common in semi-empirical schemes for computation of turbulent flows (see Monin and Yaglom, 1971) to model the turbulent flux of a passive scalar admixture $C = \bar{C} + c$, $\bar{c} = 0$, by simple gradient transport

$$\overline{cu_i} = -K_{ij}\bar{C}_{,j} \quad (1)$$

even in *inhomogeneous* situations. That is, one writes in an inhomogeneous flow

$$(\overline{cu_i})_{,i} = - (K_{ij}\bar{C}_{,j})_{,i} \quad (2)$$

The transport coefficient K_{ij} may be variously determined from local or global turbulent quantities.

The form (1) or (2) is strictly correct even in kinetic theory only in a homogeneous situation, and it is not *à priori* clear that retaining K_{ij} inside the divergence in (2) gives the proper lowest-order correction for inhomogeneity*. In fact, we shall attempt to show that it does not.

First, let us present an argument of Kolmogorov (Monin and Yaglom, 1971, p. 610). As originally presented, this argument related specifically to a Markov process, having anisotropic transport coefficient. We will

* For a general discussion of application of gradient transport forms to turbulent transport, see Corrsin (1974). We are concerned here not with their general inapplicability, but with finding the correct kinetic theory form in inhomogeneous situations. Corrsin discusses these questions also, and beginning from a form somewhat less general than (3), he finds something similar to (9), but lacking several terms.

present a simplified one-dimensional generalization of the argument, which is not dependent on the Markov assumption.

Suppose that, at $t = 0$, each point κ on a line has an indelible concentration $C(\kappa, 0)$. The points begin to move under the action of some agency, and at time t the point originally at $\kappa, 0$ is found at X, t . Let $P(X, t/\kappa, 0)dX$ be the probability that a point beginning from $\kappa, 0$ is found at time t between X and $X+dX$. Then the proportion of the line segment $(\kappa, \kappa+d\kappa)$ to arrive between X and $X+dX$ is $P(X, t/\kappa, 0)dXd\kappa$. Now, at the time t , the total number of points which have crossed to the right of an arbitrary point, κ_0 , will be those which have positions on the right at t , but were on the left at 0 . The net integrated flux to the right will be the difference between those that have moved to the right and those that have moved to the left. The mean net integrated flux of contaminant will be given by weighting each point by its corresponding concentration, thus:

$$F = \int_{-\infty}^{\kappa_0} d\kappa \int_{\kappa_0}^{\infty} C(\kappa, 0) P(X, t/\kappa, 0) dX - \int_{\kappa_0}^{\infty} d\kappa \int_{-\infty}^{\kappa_0} C(\kappa, 0) P(X, t/\kappa, 0) dX \quad (3)$$

The flux at time t can be obtained by taking the time-derivative after the expression has been evaluated. We may make a change of variables to

$$\kappa - \kappa_0 = Z, \quad X - \kappa = \zeta \quad (4)$$

and reverse the order of integration to give

$$\begin{aligned}
 F = & \int_0^{\infty} d\zeta \int_{-\zeta}^0 dZ C(\kappa_0 + Z, 0) P(\kappa_0 + Z + \zeta, t/\kappa_0 + Z, 0) \\
 & - \int_{-\infty}^0 d\zeta \int_0^{-\zeta} dZ C(\kappa_0 + Z, 0) P(\kappa_0 + Z + \zeta, t/\kappa_0 + Z, 0)
 \end{aligned} \quad (5)$$

Now, the integrand may be considered as a function of Z , and expanded in a Taylor series about κ_0 (presuming that it is suitably well behaved):

$$C(Z + \kappa_0, 0) P(\kappa_0 + Z + \zeta, t/\kappa_0 + Z, 0) = \sum_{n=0}^{\infty} \frac{1}{n!} Z^n \frac{\partial^n}{\partial \kappa_0^n} [C(\kappa_0, 0) P(\kappa_0 + \zeta, t/\kappa_0, 0)] \quad (6)$$

So that the integrated flux may be written as

$$\begin{aligned}
 F = & \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} \frac{\partial^n}{\partial \kappa_0^n} [C(\kappa_0, 0) \int_{-\infty}^{+\infty} \zeta^{n+1} P(\kappa_0 + \zeta, t/\kappa_0, 0) d\zeta] \\
 = & \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} \frac{\partial^n}{\partial \kappa_0^n} [C(\kappa_0, 0) \zeta^{\overline{n+1}}]
 \end{aligned} \quad (7)$$

The flux is given by the time derivative -

$$\dot{F} = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} \frac{\partial^n}{\partial \kappa_0^n} [C(\kappa_0, 0) \zeta^{\overline{n+1}}] \quad (8)$$

This is a generalization of the form given by Kolmogorov, which stops at second order -

$$\dot{F} = C(\kappa_0, 0) \frac{d\bar{\zeta}(t)}{dt} - \frac{1}{2} \frac{\partial}{\partial \kappa_0} [C(\kappa_0, 0) \overline{\frac{d\zeta^2(t)}{dt}}] + \dots \quad (9)$$

This clearly reduces to the classical form in a homogeneous situation. It might be thought that (9) could be obtained more simply by using the fact that $C(X, t) = C(\kappa, 0)$, and expanding in series. However, this gives expressions which are easy to evaluate only in homogeneous (reversible) situations.

We must pause for a moment to discuss the relation between $C(\kappa_0, 0)$ and $\bar{C}(\kappa, t)$. In fact, $C(\kappa_0, 0) = \bar{C}(\kappa_0, 0) + c(\kappa, 0)$; since there is a flux of C , c and the fluctuating velocity u must be correlated (presuming that the c are the result of previous turbulent transport). We may expect, however, that after sufficient time (which we must define) ζ and c will become statistically independent. The time required is presumably of the order of an integral time scale in a homogeneous flow. In an inhomogeneous flow, we may expect $\overline{\zeta^2}$ to approach a constant only under very special circumstances; we may still expect, however, a distinct initial phase characterized by rapid change, followed by a phase of much slower change, the time of transition from one to the other being of the order of the current value of $\overline{\zeta^2}/2\overline{u^2}$ (where $\overline{u^2}$ is the mean square fluctuating velocity) and playing the role of an integral time scale. This is roughly the time required for ζ to lose dependence on the fluctuation c . Hence, after a time of this order, $\dot{F}$ may be averaged over the initial concentration field, resulting in the simple replacement of $C(\kappa_0, 0)$ by $\bar{C}(\kappa_0, 0)$. After a time of this order, in fact, the process may

be restarted, so that $\dot{\bar{F}}$ always depends on $\bar{C}$ at a time earlier by the (integral) time scale. Thus, in replacing $\bar{C}$ by the current value, we are supposing that $(D\bar{C}/Dt)T \ll \bar{C}$ (where T is the time scale); this is true in kinetic theory, but of course, not true in turbulence. It is, however, consistent with the complementary assumption that the length scales of the dispersion process are small relative to those of the $\bar{C}$ distribution.

Monin and Yaglom (1971) compare (9) with the more usual form

$$\dot{\bar{F}} = -\frac{1}{2} \frac{\partial C(\kappa_0, 0)}{\partial \kappa_0} \overline{\frac{d\zeta^2(t)}{dt}} \quad (10)$$

and conclude that

$$\frac{\dot{\bar{\zeta}}}{\bar{\zeta}} = \frac{1}{2} \frac{\partial}{\partial \kappa_0} \frac{\dot{\bar{\zeta}}^2}{\bar{\zeta}^2} \quad (11)$$

It does not appear that this reasoning can be correct, since it results from comparison of, effectively, the form (9) specialized to a homogeneous situation, and the full form. We shall show, however, that a form similar to (11), with a different coefficient, may well be correct.

First, we must discuss the possible value of $\frac{\dot{\bar{\zeta}}}{\bar{\zeta}}$ in a homogeneous flow. Let us consider, for example, vertical transport in an incompressible, horizontal homogeneous shear flow, without gravity. The flow must be symmetric about horizontal planes, and hence $\frac{\dot{\bar{\zeta}}}{\bar{\zeta}}, \frac{\dot{\bar{\zeta}}^3}{\bar{\zeta}^3}$, etc., must vanish. If gravity is introduced, with density fluctuations within the Boussinesq approximation (Tennekes and Lumley, 1973), we might expect to find

dissymmetry. However, we would expect to find the direction of the dissymmetry to change sign with the sign of the gravity. However, if both the sign of the density fluctuations and the sign of gravity are reversed, the equations remain unchanged. Since the entire detailed velocity field remains unchanged, the sign of $\dot{\zeta}$ cannot change. Hence it must be zero. Hence, $\dot{\zeta}$ must be zero in a homogeneous flow, as expected.

This suggests that an expression for $\dot{\zeta}$ may be obtained by considering the departure from homogeneity represented by, for example, expressions such as (11), which will vanish when the field becomes homogeneous.

It is very instructive to consider a somewhat restricted case. Let $f(t)$ be a stationary random function with zero mean and finite, non-vanishing integral scales (Lumley 1972). Let $\zeta(\kappa, t)$ be the displacement at t of the point initially at κ . Suppose that the moving point is governed by

$$\begin{aligned} \frac{d\zeta}{dt} &= F(\kappa + \zeta)f(t) & \zeta(\kappa, 0) &= 0 \\ F(Z) &= aZ^\alpha, & 0 < \alpha < 1 \end{aligned} \tag{12}$$

That is, the Lagrangian velocity can be reduced to a stationary function by renormalization. This is by no means the most general form - we could, for example, consider a case in which not the amplitude of the velocity, but the time scale, were stretched according to the location. This does not give a solvable case, however. The most general case, of course, is that in which the position and time effects are not separable.

If we define $\kappa + \zeta = Z$, and

$$\tau = \int_0^t f(t') dt' \quad (13)$$

we can write

$$\zeta = -\kappa + \kappa \left[1 + \frac{\tau}{\mu} \right]^{\frac{1}{1-\alpha}} \quad (14)$$

$$\mu = \frac{\kappa}{a(1-\alpha)}$$

where, for large time, τ is a Gaussian variable (Lumley, 1972)

$$\overline{\tau^2} \equiv 2f'^2 T, \quad \bar{\tau} = 0 \quad (15)$$

where T is the integral time scale of f , and f'^2 is its variance. Expanding the binomial in (14) we have (with $n = 1/(1-\alpha)$)

$$\bar{\zeta} = \kappa \frac{n(n-1)}{2} \frac{\overline{\tau^2}}{\mu^2} + \dots \quad (16)$$

$$\overline{\zeta^2} = \kappa^2 n^2 \frac{\overline{\tau^2}}{\mu^2} + \dots$$

Since $1-\alpha > 0$, μ is monotone increasing in κ ; the series (16) proceed in inverse powers of μ , and hence, for larger values of κ , higher order terms are less important. As $\kappa \rightarrow \infty$, the leading term is

$$\frac{\frac{1}{2} \frac{\partial \overline{\zeta^2}}{\partial \kappa}}{\bar{\zeta}} = 2 + \dots \quad (17)$$

i.e. - for very large κ , when the situation is almost homogeneous, we have

$$\frac{\dot{\zeta}}{\zeta} = \frac{1}{4} \frac{\partial}{\partial \kappa} \frac{\dot{\zeta}^2}{\zeta^2} \quad (18)$$

and this is true regardless of the value of α (so long as $0 < \alpha < 1$). The series (16) of course, terminates if $1/1-\alpha = n$ is an integer. For example, if $\alpha = 1/2$, we have

$$\begin{aligned} \frac{1}{2} \frac{\partial \dot{\zeta}^2}{\partial \kappa} &= a^2 \overline{f'^2} T \\ \frac{\dot{\zeta}}{\zeta} &= \frac{a^2}{2} \overline{f'^2} T \end{aligned} \quad (19)$$

while if $\alpha = \frac{2}{3}$,

$$\begin{aligned} \frac{\dot{\zeta}}{\zeta} &= \kappa^{1/3} \frac{a^2}{3} 2 \overline{f'^2} T \\ \frac{1}{2} \frac{\partial \dot{\zeta}^2}{\partial \kappa} &= 2 \frac{\dot{\zeta}}{\zeta} + \frac{80}{27} a^4 t T^2 \overline{f'^2}^2 \kappa^{-1/3} \end{aligned} \quad (20)$$

$\alpha = 1/2$ is the only value for which both $\frac{\dot{\zeta}}{\zeta}$ and $\partial \dot{\zeta}^2 / \partial \kappa$ are constant in time. For all others there is also a time limitation - roughly translated as requiring that total dispersion must remain small enough for the inhomogeneity across the dispersed material to remain weak.

If we accept (18) as a general value, then (9) should be

$$\dot{F} = -\frac{1}{2} \frac{\dot{\zeta}^2}{\zeta^2} \frac{\partial}{\partial \kappa_0} \overline{C}(\kappa_0, t) - \frac{1}{4} \overline{C}(\kappa_0, t) \frac{\partial}{\partial \kappa_0} \frac{\dot{\zeta}^2}{\zeta^2} + \dots \quad (21)$$

To lowest order.

That is: there is, in addition to the gradient transport form, even within the framework of kinetic theory, a convective transport term in inhomogeneous situations. In turbulence modeling, the form (21) provides a means for estimating the convection velocity; such a term has been suggested by many authors (e.g. Townsend, 1956), but without useful suggestions for estimating the form of the term.

Equation (21) of course may be generalized to several dimensions as

$$\dot{F}_i = -\frac{1}{2} \overline{\dot{\zeta}_i \zeta_j} \bar{C}_{,j}(\kappa, t) - \frac{1}{4} \bar{C}(\kappa, t) \frac{\partial}{\partial \kappa_j} (\overline{\dot{\zeta}_i \zeta_j}) \quad (22)$$

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7. EULERIAN AND LAGRANGIAN TIME MICROSCALES IN ISOTROPIC TURBULENCE

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Abstract

In isotropic "box" turbulence without a mean flow, the Lagrangian frequency spectrum extends to frequencies of the order $(\epsilon/\nu)^{1/2}$ (ϵ is the dissipation rate of kinetic energy per unit mass, ν is the kinematic viscosity of the fluid). This leads to an estimate that makes the rms value of du/dt of order $(\epsilon^3/\nu)^{1/4}$. The Eulerian frequency spectrum, however, extends to higher frequencies than its Lagrangian counterpart; this is caused by spectral broadening associated with large-scale advection of dissipative eddies. As a consequence, the rms value of $\partial u/\partial t$ at a fixed observation point is (apart from a numerical factor) $R_\lambda^{1/2}$ times as large as the rms value of du/dt (R_λ is the turbulence Reynolds number based on the Taylor microscale). The results of a theoretical analysis based on these premises agree closely with data obtained by Comte-Bellot and Corrsin. The analysis also suggests that the Eulerian frequency spectrum has a $\omega^{-5/3}$ behavior in the inertial subrange, and that it is not governed by Kolmogorov similitude.

1. Introduction

The study of turbulent diffusion requires that the distinction between Eulerian statistics (those obtained by sensors at fixed locations) and Lagrangian statistics (pertaining to the motion of fluid particles, aerosols and pollutants) be kept in focus at all times. Diffusion is a Lagrangian process, and there is no one-to-one correspondence between Lagrangian variables and their Eulerian counterparts. This paper reports on the distinctive differences between Eulerian and Lagrangian frequency spectra.

The shapes of the Eulerian and Lagrangian frequency spectra in isotropic "box" turbulence without mean flow have been subjects of some speculation over the years (Inoue 1951, Corrsin 1963, Tennekes and Lumley 1972). Both spectra are assumed to obey Kolmogorov scaling; this leads to forms which are proportional to $\epsilon\omega^{-2}$ in the inertial subrange (ϵ is the dissipation rate of kinetic energy per unit mass, ω is the angular velocity).

Comte-Bellot and Corrsin (1971) measured the Eulerian time correlation function (in a frame of reference moving with the mean flow) of isotropic wind-tunnel turbulence. From their experimental results, they calculated

the Eulerian time microscale. The calculated value, however, was five times as small as the one derived from the hypothetical similarity between the Eulerian and Lagrangian frequency spectra. This discrepancy suggests that the assumptions involved in the theoretical models should be reexamined. In this paper, the results of an alternative theoretical approach are presented.

The highest frequencies characterizing the dynamics of turbulence occur at the smallest length scales. The Kolmogorov microscale is $(\nu^3/\epsilon)^{1/4}$, the Kolmogorov frequency of dissipative eddies is $(\epsilon/\nu)^{1/2}$, and the kinetic energy of the dissipative eddies is of order $(\nu\epsilon)^{1/2}$ per unit mass. It appears reasonable to postulate that the position of the viscous cut-off in the Lagrangian frequency spectrum is determined by the parameters ν and ϵ .

An Eulerian observer of "box" turbulence, however, will on occasion encounter appreciable energy at frequencies much larger than $(\epsilon/\nu)^{1/2}$. Random advection of the dissipative structure past the observation point causes spectral broadening, which is not unlike a Doppler effect. The highest frequencies that will be observed must be associated with the advection of dissipative eddies past the observation point by the most energetic eddies. The frequencies involved must be of order q/η , where $1/2(q^2)$ is the mean kinetic energy per unit mass and η is the Kolmogorov microscale $(\nu^3/\epsilon)^{1/4}$. A simple calculation, based on the assumption that $\epsilon \sim q^3/\ell$ (where ℓ is an integral scale), shows that q/η is larger than $(\epsilon/\nu)^{1/2}$ by a factor proportional to $Re_\ell^{1/4} = (q\ell/\nu)^{1/4}$.

In turbulence at high Reynolds numbers, therefore, the dissipative eddies flow past an Eulerian observer in much less time than the time scale which characterizes their own dynamics. This suggests that G. I. Taylor's "frozen-turbulence" approximation should be valid in the analysis of the consequences of large-scale advection of the turbulent microstructure. Since Eulerian frequencies larger than $(\epsilon/\nu)^{1/2}$ can be generated only by advective spectral broadening, and since the rms value of $\partial u/\partial t$ is determined by the position of the viscous cut-off in the Eulerian frequency spectrum, it appears reasonable to postulate that the Eulerian time microscale is determined by large-scale advection of dissipative eddies. This hypothesis serves as the starting point for further analysis.

2. Analysis

If Taylor's hypothesis governs the advection of dissipative eddies past a fixed observation point, we can write

$$\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x} - v \frac{\partial u}{\partial y} - w \frac{\partial u}{\partial z} \quad (1)$$

If we assume that the microstructure is statistically independent of the

energy-containing eddies, we obtain for the mean-square value of (1) in isotropic turbulence without mean flow

$$\overline{\left(\frac{\partial u}{\partial t}\right)^2} = \overline{u^2 \left(\frac{\partial u}{\partial x}\right)^2} + \overline{v^2 \left(\frac{\partial u}{\partial y}\right)^2} + \overline{w^2 \left(\frac{\partial u}{\partial z}\right)^2} . \quad (2)$$

In isotropic turbulence, we have (Batchelor, 1953)

$$\overline{u^2} = \overline{v^2} = \overline{w^2} , \quad (3)$$

$$\overline{\left(\frac{\partial u}{\partial x}\right)^2} = \frac{1}{2} \overline{\left(\frac{\partial u}{\partial y}\right)^2} = \frac{1}{2} \overline{\left(\frac{\partial u}{\partial z}\right)^2} . \quad (4)$$

Therefore, (2) reduces to

$$\overline{\left(\frac{\partial u}{\partial t}\right)^2} = 5 \overline{u^2 \left(\frac{\partial u}{\partial x}\right)^2} . \quad (5)$$

In isotropic turbulence, the following relation holds (Tennekes and Lumley 1972):

$$\epsilon = 15\nu \overline{\left(\frac{\partial u}{\partial x}\right)^2} \quad (6)$$

Also, the Taylor microscale λ is defined by

$$\overline{\left(\frac{\partial u}{\partial x}\right)^2} = \frac{\overline{u^2}}{\lambda^2} . \quad (7)$$

Therefore, (5) may be written as

$$\overline{\left(\frac{\partial u}{\partial t}\right)^2} = \frac{1}{3} \overline{u^2} \frac{\epsilon}{\nu} , \quad (8)$$

or as

$$\overline{\left(\frac{\partial u}{\partial t}\right)^2} = 5 \frac{\overline{(u^2)^2}}{\lambda^2} . \quad (9)$$

Comte-Bellot and Corrsin (1971) define the Eulerian time microscale τ_E through the relation

$$\overline{\left(\frac{\partial u}{\partial t}\right)^2} = \frac{2\overline{u^2}}{\tau_E^2} . \quad (10)$$

Substitution of (9) into (10) yields

$$\tau_E = \left\{ \frac{8\lambda^2}{20 \overline{u^2}} \right\}^{1/2} . \quad (11)$$

In the experiments by Comte-Bellot and Corrsin, the value of τ_E was determined from the Eulerian time correlation behind a two-inch grid, with the origin of the time delay chosen at the point $x/M = 42$ (M is the mesh size of the grid). Their experimental value for τ_E was 6.2 milliseconds. At the reference position, λ was equal to 0.484 cm and $(u^2)^{1/2}$ was 22.2 cm sec^{-1} . Substituting these values into (11), we find that the predicted value of τ_E is 14 milliseconds.

If τ_E is estimated on basis of the hypothetical similarity between the Eulerian and Lagrangian frequency spectra (Corrsin 1963), a value of approximately 30 milliseconds is obtained (Comte-Bellot and Corrsin 1971). It appears that calculations based on the advection hypothesis are more realistic than calculations based on the Eulerian-Lagrangian similarity hypothesis. It should be pointed out, however, that the low Reynolds number grid turbulence used in the Comte-Bellot and Corrsin experiments is not an ideal test case for the advection hypothesis. At low Reynolds numbers, the advective spectral broadening is not very pronounced, and the validity of Taylor's hypothesis is questionable. Still, the relatively good agreement between the prediction based on the advection hypothesis and the experimental result is sufficiently encouraging to attempt an alternative analysis of the Eulerian frequency spectrum in "box" turbulence.

3. The Eulerian Frequency Spectrum

The frequency spectrum observed at a fixed point in isotropic turbulence without a mean flow is strongly affected by advective spectral broadening. At a frequency corresponding to the viscous cut-off in the Lagrangian time spectrum for example, fluctuations are observed which are related to the passage of eddies in the inertial subrange. Some qualitative estimates will help to illustrate the issue. Large-scale advection of eddies of size r (where r is taken to be in the inertial subrange) creates frequencies of order q/r . In order to find the value of r that contributes most to the energy at the cut-off frequency $(\epsilon/\nu)^{1/2}$ of the Lagrangian spectrum, we have to put

$$q/r \sim (\epsilon/\nu)^{1/2} . \quad (12)$$

This yields

$$r \sim q(\nu/\epsilon)^{1/2} . \quad (13)$$

If r relates to an eddy in the inertial subrange, its kinetic energy may be estimated as (Tennekes and Lumley, 1972)

$$\frac{1}{2} u^2(r) \sim \epsilon^{2/3} r^{2/3} . \quad (14)$$

The contribution of these eddies to the kinetic energy at the Eulerian frequency $(\epsilon/\nu)^{1/2}$ is therefore

$$\frac{1}{2} u^2(r, (\epsilon/\nu)^{1/2}) \sim \epsilon^{1/3} q^{2/3} \nu^{1/3}. \quad (15)$$

In the absence of advection by large scales, the kinetic energy at frequency $(\nu/\epsilon)^{1/2}$ would be

$$\frac{1}{2} u^2(\eta, (\epsilon/\nu)^{1/2}) \sim (\nu\epsilon)^{1/2}. \quad (16)$$

The ratio of (15) and (16) is

$$\frac{\frac{1}{2} u^2(r, (\epsilon/\nu)^{1/2})}{\frac{1}{2} u^2(\eta, (\epsilon/\nu)^{1/2})} \sim \left(\frac{q^2}{(\epsilon\nu)^{1/2}} \right)^{1/3}. \quad (17)$$

Here, $(\epsilon\nu)^{1/2}$ is the kinetic energy of the dissipative eddies. Clearly, the advective contribution outweighs the quasi-Lagrangian one, at least if the Reynolds number of the turbulence is large enough.

We conclude that the high-frequency end of the Eulerian time spectrum must be dominated by the Doppler shifts in frequency caused by random advection by the energy-containing eddies. This generalization of the advection hypothesis permits us to obtain a probable form of the inertial subrange (obviously better referred to as the inertial-advective subrange) in the Eulerian frequency spectrum.

If the dominant contribution to the kinetic energy at a frequency ω in the inertial-advective subrange is made by large-scale advection of eddies in the inertial subrange of the wave-number spectrum, we have

$$\omega \sim q/r, \quad (18)$$

and

$$\frac{1}{2} u^2(\omega) \sim \epsilon^{2/3} r^{2/3}. \quad (19)$$

Substitution of (18) into (19) yields

$$\frac{1}{2} u^2(\omega) \sim \epsilon^{2/3} q^{2/3} \omega^{-2/3}. \quad (20)$$

The Eulerian frequency spectrum is defined as the kinetic energy per unit frequency. We obtain

$$\Phi_E(\omega) = \beta_E \epsilon^{2/3} q^{2/3} \omega^{-5/3}, \quad (21)$$

where β_E is an unknown constant, which presumably is of order one.

The inertial-advective subrange in the Eulerian frequency spectrum thus does not obey Kolmogorov scaling, and is markedly different from the inertial subrange in the Lagrangian frequency spectrum. The latter is (Inoue 1951, Corrsin 1963, Tennekes and Lumley 1972)

$$\phi_L(\omega) = \beta_L \epsilon \omega^{-2}. \quad (22)$$

Let us compare (21) and (22) at the lowest frequency for which they might give a reasonable representation. That frequency is $\omega \sim q/\ell$ (ℓ is an integral scale), and we find

$$\frac{\phi_E(q/\ell)}{\phi_L(q/\ell)} = \frac{\beta_E}{\beta_L} \left(\frac{q^3/\ell}{\epsilon} \right)^{1/3}. \quad (23)$$

Since $\epsilon \sim q^3/\ell$, the values of ϕ_E and ϕ_L at the large-scale end are of comparable magnitude. In the absence of high Reynolds number data on these spectra, we cannot determine if the Eulerian spectrum is likely to have a ω^{-2} shape at frequencies below those in the inertial-advective subrange, but it seems fair to speculate that such a small difference in spectral slope would be extremely hard to verify experimentally. One point appears to be clear, however: since the spectral "smearing" caused by random advection tends to remove discontinuities in the spectral slope, the inertial-advective spectrum proposed here may well be a valid approximation at frequencies near those characteristic of the large-scale structure.

The spectra given by (21) and (22) can, after multiplication by ω^2 , be integrated to obtain estimates for the mean-square values of $\partial u/\partial t$ and du/dt :

$$\begin{aligned} \overline{\left(\frac{\partial u}{\partial t}\right)^2} &= \int_0^\infty \omega^2 \phi_E(\omega) d\omega = \int_0^\infty \beta_E \epsilon^{2/3} q^{2/3} \omega^{1/3} d\omega \\ &\equiv \frac{3}{4} \beta_E \epsilon^{2/3} q^{2/3} \omega_{E,D}^{4/3}, \end{aligned} \quad (24)$$

and

$$\begin{aligned} \overline{\left(\frac{du}{dt}\right)^2} &= \int_0^\infty \omega^2 \phi_L(\omega) d\omega = \int_0^\infty \beta_E \epsilon d\omega \\ &\equiv \beta_E \epsilon \omega_{L,D}. \end{aligned} \quad (25)$$

Here, $\omega_{E,D}$ is the frequency of the viscous cut-off in the Eulerian spectrum, and $\omega_{L,D}$ is its Lagrangian counterpart. According to the advection hypothesis,

$$\omega_{E,D} = \frac{q}{\eta} = q \epsilon^{1/4} \nu^{-3/4}, \quad (26)$$

while the highest Lagrangian frequency is

$$\omega_{L,D} = (\epsilon/\nu)^{1/2}. \quad (27)$$

In (26) and (27), unknown numerical coefficients have been ignored. Substitution of (26) into (24) yields

$$\overline{\left(\frac{\partial u}{\partial t}\right)^2} = C_E^2 q^2 \left(\frac{\epsilon}{\nu}\right); \quad (28)$$

The value of C_E can be estimated by comparing (28) with (8); this yields $C_E = 1/3$, because $q^2 = 3 \overline{u^2}$.

Substitution of (27) into (25) yields

$$\overline{\left(\frac{du}{dt}\right)^2} = C_L^2 \left(\frac{\epsilon^3}{\nu}\right)^{1/2}. \quad (29)$$

The value of C_L can be estimated from the data given by Shlien and Corrsin (1974). They define the Lagrangian time microscale by

$$\overline{\left(\frac{du}{dt}\right)^2} = \frac{2\overline{u^2}}{\tau_L^2}. \quad (30)$$

Substitution of (30) into (29) gives

$$\tau_L = \frac{2^{1/2} \overline{(u^2)}^{1/2}}{C_L (\epsilon^3/\nu)^{1/4}}. \quad (31)$$

For $\overline{(u^2)}^{1/2} = 22.2 \text{ cm sec}^{-1}$, $\epsilon = 0.4740 \text{ m}^2 \text{ sec}^{-3}$ and $\nu = 15 \times 10^{-6} \text{ m}^2 \text{ sec}^{-1}$, Shlien and Corrsin found $\tau_L = 76 \times 10^{-3} \text{ sec}$. Substitution of these values into (31) gives $C_L \cong 4/9$ approximately.

The ratio between the Eulerian time microscale and its Lagrangian counterpart thus is given by (note that Corrsin's definition of τ_E , given in (10), involves a factor 4, whereas his definition of τ_L , given in (30), involves a factor 2):

$$\frac{\tau_E}{\tau_L} = \frac{4}{3} \frac{(\epsilon \nu)^{1/4}}{q}. \quad (32)$$

Here we have used $C_E = 1/3$, $C_L = 4/9$.

The velocity $(\epsilon \nu)^{1/4}$ occurring in (32) is the Kolmogorov velocity of the dissipative eddies. Since the ratio $(\epsilon \nu)^{1/4}/q$ is proportional to $R_\ell^{-1/4} = (q\ell/\nu)^{-1/4}$, this result confirms that the Eulerian time microscale must be appreciably smaller than its Lagrangian counterpart if the Reynolds number of the turbulence is large enough. The comparison also shows that the approximate equality of τ_E and τ_L predicted by Corrsin's (1963) Eulerian-Lagrangian similarity hypothesis is bound to produce unrealistic

values of τ_E . The values of τ_E and τ_L obtained in the experiments by Corrsin and his co-workers prove that the advection hypothesis is justified, even at relatively low Reynolds numbers.

4. Discussion

The consequences of the advection hypothesis are rather embarrassing in a personal sense. The section on time spectra in Chapter 8 of Tennekes and Lumley (1972) treats the Eulerian spectrum on basis of the similarity hypothesis; if the analysis presented in this paper proves to be reliable, that section will have to be revised before a new edition goes to press.

The advection-dominated Eulerian spectrum strongly suggests that the evolution of turbulence in wave-number space is best computed on a Lagrangian basis. Large-scale advection of the small-scale structure creates Eulerian Fourier components at frequencies that are higher than the angular velocities characterizing the internal evolution of the scales being advected, and calculations of the temporal evolution at the points of an Eulerian grid would tend to get overwhelmed by these spurious advection effects. From this point of view, models such as Kraichnan's Lagrangian-history, direct-interaction approximation obviously are to be preferred above their Eulerian counterparts.

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8. NOTES ON TURBULENT FLOW IN TWO AND THREE DIMENSIONS

by

H. Tennekes

1. Introduction

These notes contain the core material for a paper that will be submitted for publication in the near future. Though the issues taken up in these notes do not pertain directly to the atmospheric diffusion modeling tasks of the Select Research Group, it is felt that the analysis presented here contributes to the study of some of the problems we face in our research.

The dispersion of atmospheric pollutants is affected by motions on all scales, ranging from the turbulence microstructure in the mixed layer to mesoscale and synoptic-scale flow patterns. The study of three-dimensional turbulence needs to be related to that of the quasi two-dimensional "turbulence" of the synoptic eddies, if only to obtain a more profound insight into the extremely difficult task of modeling mesoscale motions, for which neither the assumptions used in turbulence theory nor the approximations employed in synoptic analysis are valid.

This material is based on lectures in the author's turbulence course; it was presented also at a seminar for the Department of Meteorology given in the spring of 1974.

2. Statement of the Issue

What do a turbulence theoretician and a numerical modeler of atmospheric motions have in common? It would seem that there is not much that unites them. The turbulence researcher ordinarily takes a statistical approach to his flows, but the forecaster treats his flows in a deterministic way. What is it that makes the turbulence community prefer statistics? And what happens when you think of an ensemble of synoptic flow fields as a kind of turbulence? A forecaster identifies "eddies" (such as a low-pressure system) on the weather map with great confidence, but the turbulence researcher has a hard time recognizing individual eddies. Why is that so? Is it the limited spatial resolution of a synoptic analysis that makes a weather map so clean-looking, or do synoptic flows in fact have much less microstructure than the kind of flow that is found in the atmospheric boundary layer?

Questions such as these can be answered only if one is willing to study the "primitive equations". These provide a common foundation, and

we trust that they are capable of providing pertinent insight. In our exploration, we shall emphasize the role of vorticity, since it holds a key position both in turbulence dynamics and in dynamical meteorology. We restrict the analysis to incompressible flows. By doing so we cannot do justice to the energetics of atmospheric flows; however, we can take a close look at major kinematical aspects. The generalization of the equations of motion to stratified fluids in an environment exposed to the acceleration of gravity is discussed in textbooks on dynamical meteorology (for example, Haltiner and Martin).

3. The Equations of Motion

For our purposes, it is useful to write the Navier-Stokes equations in such a way that the role of vorticity is emphasized. The formulation we select is (Tennekes and Lumley, p. 77)

$$\frac{\partial u_i}{\partial t} = -\frac{1}{\rho} \frac{\partial}{\partial x_i} \left(p + \frac{1}{2} \rho u_j u_j \right) + \epsilon_{ijk} u_j \omega_k - \nu \epsilon_{ijk} \frac{\partial \omega_k}{\partial x_j} . \quad (1^a)$$

In vector notation, this reads

$$\frac{\partial \underline{u}}{\partial t} = -\frac{1}{\rho} \nabla \left(p + \frac{1}{2} \rho \underline{u} \cdot \underline{u} \right) + \underline{u} \times \underline{\omega} - \nu \nabla \times \underline{\omega} . \quad (1^b)$$

Local accelerations apparently are caused by the gradient of the stagnation pressure (the validity of Bernoulli's equation in steady flow without vorticity is evident here), by the "vortex force" $\underline{u} \times \underline{\omega}$, and by the viscous force (the last term of (1), which shows that in solid-body rotation the viscous force is zero).

The most interesting of these forces is the vortex force $\underline{u} \times \underline{\omega}$. Since its direction is normal to the velocity vector, this force does not perform work; therefore, the vortex force does not affect the kinetic energy of the flow in an explicit way. Nevertheless, the vortex force plays a dominant role in the evolution of many flow fields.

Equation (1) is written for an inertial frame of reference. If it is to be used in a rotating coordinate system, the vortex force has to be replaced by

$$\underline{u} \times \underline{\omega}_a = \underline{u} \times \underline{\omega}_r + 2\underline{u} \times \underline{\Omega} . \quad (2)$$

Here, $\underline{\omega}_a$ is the "absolute" vorticity, $\underline{\omega}_r$ is the "relative" vorticity, and $\underline{\Omega}$ is the angular velocity of the coordinate system. The factor 2 in the last term occurs because vorticity is defined as twice the angular velocity of a small fluid element. In the conversion to a rotating frame we also should include the centrifugal force, but that can be incorporated in the definition of the pressure p (see, for example, Greenspan's book).

One major difference between turbulence and synoptic flows is that for large-scale atmospheric motions the "external" vortex force (the Coriolis force) tends to control the evolution of the flow field, while in fully three-dimensional flows such as turbulence the "internal" vortex force plays a major role. For example, the shear-stress components of the Reynolds stress tensor in turbulence are associated with the contributions of turbulent velocity and vorticity fluctuations to the average vortex force acting on the mean flow (Tennekes and Lumley, p. 79).

In a two-dimensional flow field evolving on a horizontal plane, the vertical component of the velocity is zero and so are both of the horizontal components of vorticity. Defining $\underline{v}$ as the horizontal wind speed vector, ∇_h as the horizontal gradient operator, ζ as the relative vorticity, f as the vertical component of 2Ω (f is the Coriolis parameter), and $\underline{k}$ as the vertical unit vector, we find that (1) reduces to

$$\frac{\partial \underline{v}}{\partial t} = -\frac{1}{\rho} \nabla_h (p + \frac{1}{2} \rho \underline{v} \cdot \underline{v}) + \underline{v} \times \underline{k} \zeta + \underline{v} \times \underline{k} f. \quad (3)$$

In this equation we have ignored the viscous force.

The geostrophic wind $\underline{v}_g$ is defined by

$$-\frac{1}{\rho} \nabla_h p = -\underline{v}_g \times \underline{k} f. \quad (4)$$

With this relation, (3) may be rewritten as

$$\frac{\partial \underline{v}}{\partial t} = -\frac{1}{\rho} \nabla_h (\frac{1}{2} \rho \underline{v} \cdot \underline{v}) + \underline{v} \times \underline{k} \zeta + (\underline{v} - \underline{v}_g) \times \underline{k} f. \quad (5)$$

4. Order-of-Magnitude Estimates

For large-scale motions in the earth's atmosphere, the two terms of equation (4) are of order $10^{-3} \text{ msec}^{-2}$:

$$\frac{1}{\rho} \nabla_h p \text{ and } \underline{v}_g \times \underline{k} f \sim 10^{-3} \text{ msec}^{-2}. \quad (6)$$

The terms of (5), however, generally are one order of magnitude smaller:

$$\frac{\partial \underline{v}}{\partial t}, \nabla_h (\frac{1}{2} \underline{v} \cdot \underline{v}), \underline{v} \times \underline{k} \zeta, (\underline{v} - \underline{v}_g) \times \underline{k} f \sim 10^{-4} \text{ msec}^{-2}. \quad (7)$$

These estimates imply that the relative vorticity ζ is about 10 times as small as f , so that its order of magnitude is 10^{-5} sec^{-1} . Also, the ageostrophic wind component $\underline{v} - \underline{v}_g$ is implied to be about 10 times as small as $\underline{v}_g$. With $\underline{v}_g \sim 10 \text{ msec}^{-1}$, this means that $\underline{v} - \underline{v}_g \sim 1 \text{ msec}^{-1}$.

What would be the orders of magnitude of the various terms in the equations of motion if they were used to describe a three-dimensional turbulent flow with the same velocity and length scales? In 3D turbulence, most of the vorticity resides at very small scales, and the mean-square vorticity (twice the "enstrophy") is given by

$$\overline{\omega_i \omega_i} = \overline{\underline{\omega} \cdot \underline{\omega}} = \epsilon/\nu, \quad (8)$$

where ϵ is the mean dissipation rate of kinetic energy per unit mass, and ν (as before) is the kinematic viscosity of the fluid. The dissipation rate may be estimated as (Tennekes and Lumley, p. 20)

$$\epsilon \sim u^3/L, \quad (9)$$

where u is a velocity characteristic of the large-scale eddy motion, and L is the length scale (for simplicity defined as a quarter wavelength) of the large eddies.

In order to make a fair comparison between 3D turbulence and synoptic flows, we select $u = 10 \text{ msec}^{-1}$ and $L = 10^6 \text{ m}$ ($= 1000 \text{ km}$). This choice is consistent with equations (6) and (7), because it makes the relative vorticity of the large eddies of order 10^{-5} sec^{-1} and the internal vortex force of order $10^{-4} \text{ msec}^{-2}$ if the same values of u and L are used in the equations for large-scale atmospheric flows.

With $u = 10 \text{ msec}^{-1}$ and $L = 10^6 \text{ m}$, we obtain $\epsilon \sim 10^{-3} \text{ m}^2 \text{ sec}^{-3}$, and, with $\nu = 15 \times 10^{-6} \text{ m}^2 \text{ sec}^{-1}$ for air at sea level, we obtain the following estimate for the order of magnitude of the vorticity fluctuations:

$$\omega \sim 10 \text{ sec}^{-1}. \quad (10)$$

Since $u \sim 10 \text{ msec}^{-1}$, we conclude that the internal vortex force, $\underline{u} \times \underline{\omega}$, is of order 100 msec^{-2} , which is six orders of magnitude larger than in the two-dimensional reference case.

This estimate for $\underline{u} \times \underline{\omega}$, however, is dominated by the contributions to the vortex force made by large-scale advection of small-scale vorticity fluctuations. The smallest eddy size in 3D turbulence is $\eta = (\nu^3/\epsilon)$; using the same numbers as before, this gives $\eta \sim 10^{-3} \text{ m}$ (1 mm). Advection of those eddies past a fixed observation point with velocities of order 10 msec^{-1} gives rise to angular velocities of order 10^4 sec^{-1} . This is three orders of magnitude larger than the angular velocities of those small eddies themselves (see equation (10)). If the reciprocal of ω is taken as the smallest dynamically significant time scale in the turbulence, it would seem that it isn't really necessary to carry events at smaller time scales along. If we filter all angular velocities greater than 10^{-1} sec^{-1} away, we remove the fluctuations associated with the large-scale advection of small-scale features without doing harm to the evolution of the flow. This procedure is valid only if the large-scale advection of small-scale features is governed b

$$\frac{\partial \underline{u}_s}{\partial t} + (\underline{u}_\ell \cdot \nabla) \underline{u}_s \equiv 0. \quad (11)$$

Here, $\underline{u}_s$ is the small-scale velocity and $\underline{u}_\ell$ is the large-scale velocity. Equation (11) is the "frozen-turbulence approximation", proposed originally by G. I. Taylor.

If these advection effects are removed by filtering, we still need to consider the vortex force arising from small-scale advection of small-scale vorticity. This requires that the characteristic velocity of the small-scale structure of 3D turbulence be used in estimating $\underline{u} \times \underline{\omega}$. The velocity of the smallest eddies may be estimated as $(\nu \epsilon)^{1/4}$ (Tennekes and Lumley, p. 20); with $\nu = 15 \times 10^{-6} \text{ m}^2 \text{sec}^{-1}$ and $\epsilon = 10^{-3} \text{ m}^2 \text{sec}^{-3}$, this gives $10^{-2} \text{ msec}^{-1}$. Therefore, the order of magnitude of $\underline{u} \times \underline{\omega}$ in 3D turbulence with the same velocity and length scales as synoptic flows is, when large-scale advection effects are filtered out,

$$\underline{u} \times \underline{\omega} \sim 10^{-1} \text{ msec}^{-2}. \quad (12)$$

These effects occur at angular velocities of order 10 sec^{-1} (eddy sizes near 10^{-3} m advected at relative velocities of about $10^{-2} \text{ msec}^{-1}$). Therefore, the limiting frequency corresponding to $\omega \sim 10 \text{ sec}^{-1}$ does not need to be changed.

The estimate presented in equation (12) can be supported by estimates of some of the other terms in the equations of motion. The mean-square value of du/dt in 3D turbulence is estimated from the Lagrangian time spectrum (Tennekes and Lumley, p. 279) as

$$\overline{\left(\frac{du}{dt}\right)^2} \sim \left(\frac{\epsilon^3}{\nu}\right)^{1/2}. \quad (13)$$

A different kind of calculation (Batchelor, p. 183) gives for the pressure-gradient fluctuations in turbulent flows:

$$\overline{\left(\frac{1}{\rho} \nabla p\right)^2} \sim 3 \left(\frac{\epsilon^3}{\nu}\right)^{1/2}. \quad (14)$$

If we continue to use $\epsilon \sim 10^{-3} \text{ m}^2 \text{sec}^{-3}$ and $\nu = 15 \times 10^{-6} \text{ m}^2 \text{sec}^{-1}$, we find that

$$\frac{du}{dt} \sim 10^{-1} \text{ msec}^{-2}, \quad (15)$$

$$\frac{1}{\rho} \nabla p \sim 10^{-1} \text{ msec}^{-2}. \quad (16)$$

These numbers are comparable with the estimate given in equation (12).

If large-scale advection of small-scale fluctuations had not been filtered out, we would have, from (10) and (11),

$$\frac{\partial \underline{u}}{\partial t} \sim 10^2 \text{ msec}^{-2}. \quad (17)$$

Comparing this with (15), we see that it indeed is fair to use the frozen-turbulence approximation in (11).

The Coriolis force in this turbulent flow is of order $10^{-3} \text{ msec}^{-2}$ ($u \sim 10 \text{ msec}^{-1}$, $f = 10^{-4} \text{ sec}^{-1}$). This suggests that the Coriolis force plays an altogether insignificant role in the temporal evolution of 3D turbulence. In all fairness, however, it should be pointed out that the role of the Coriolis force in the evolution of the large-scale features of 3D turbulence is not necessarily small. In order to recover the large-scale dynamics, the equations of motion have to be filtered in such a way that the rapid changes associated with the small-scale structure are removed. This is at the heart of the issues mentioned in the introduction. In 3D turbulence, the temporal changes in the flow field are dominated by the dynamics of the smallest scales of motion; if one is primarily interested in the evolution of the larger scales, one has to remove the small scales by averaging. However, as soon as averaging is performed, say over a grid with relatively coarse spacing, new unknowns are introduced into the equations of motion. These unknowns are the average subgrid-scale eddy forces, which make the system undetermined (the "closure problem" of turbulence). The only way to solve this problem is to employ parameterization techniques for the sub-grid-scale effects. In a Lagrangian frame of reference (which removes the troublesome advection effects), the temporal rate of change of 3D turbulence with the same length and velocity scales as synoptic flows is 1000 times as rapid as that of its two-dimensional counterpart. For large-scale atmospheric flows, $\bar{v} \sim 10 \text{ msec}^{-1}$ and $d\bar{v}/dt \sim 10^{-4} \text{ msec}^{-2}$, so that the characteristic time of temporal changes is of order 10^5 sec (the reciprocal of the relative vorticity ζ). This implies that in a numerical prediction scheme the time step could be at least 10^4 sec (a few hours). This estimate also suggests that, generally speaking, there is no need to draw weather maps more often than every three hours.

In the corresponding 3D flow, $du/dt \sim 10^{-1} \text{ msec}^{-2}$. Again using $u \sim 10 \text{ msec}^{-1}$, we find that the time scale becomes of order 10^2 sec (about two minutes). This is not a fair estimate, however, because du/dt is greatest for the smallest eddies. The vorticity of those eddies is of order 10 sec^{-1} (equation (10)), and if we want to include their evolution we have to use a time step of order 10^{-2} sec , and a grid spacing of 10^{-3} m . Clearly, the drawing of weather maps for 3D turbulence is an insurmountable task!

5. The Effects of Scale

The obviously quite dramatic differences between large-scale atmospheric flows and their three-dimensional counterparts can be illustrated further by a study of the effects of scale on the equations of motion. In this way, we should be able to find answers to such problems as the validity of using the equations of motion for atmospheric flows without including subgrid-scale forces associated with the averaging processes that are used in practice.

We restrict our analysis to eddy sizes that are small compared to the

dimensions of the large-scale motion. This restriction allows us to use the relatively simple formulations that have been developed for the "inertial subranges" of two- and three-dimensional turbulence.

In the inertial subrange of two-dimensional turbulence, the kinetic energy spectrum drops off as the inverse third power of the wave number (see e.g., Charney, 1971). This behavior implies that an eddy of size λ (where $\lambda \ll L$ and L is the scale of the large eddies) has a characteristic velocity which is proportional to λ . Later in this paper we shall show that a fair estimate for the velocity $v(\lambda)$ of a 2D eddy of size λ is

$$v(\lambda) \sim (L/a)f\lambda \quad (18)$$

Here, a is the earth's radius. For $\lambda \rightarrow L$, equation (18) becomes $v(L) \sim (L/a)fL$, which is of order 10 msec^{-1} if $L/a \sim 10^{-1}$, $f \sim 10^{-4} \text{ sec}^{-1}$ and $L \sim 10^6 \text{ m}$. Therefore, (18) is consistent with the numbers we used earlier.

The corresponding relative vorticity at scale λ can be estimated as $v(\lambda)/\lambda$. This yields

$$\zeta(\lambda) \sim (L/a)f \quad (19)$$

This indicates that in the inertial range of two-dimensional turbulent flows the vorticity is independent of eddy size. We note that equation (19) is consistent with the numbers used earlier: the relative vorticity is of order 10^{-5} sec^{-1} at all scales in this range of scales.

Eddies of scale λ thus make a contribution to the Coriolis force which may be estimated as

$$(\mathbf{v} \times \mathbf{k}f)_\lambda \sim (L/a)^2 f^2 \lambda \quad (20)$$

This decreases with decreasing eddy size. The geostrophic balance, equation (4), thus is not affected strongly by the presence of small eddies. This implies that the definition of the geostrophic wind does not need to be corrected for subgridscale effects if the grid size is reasonably small (say, a few hundred kilometers).

Let us now assume that the near-cancellation of pressure gradient and Coriolis force holds also in the inertial range. This assumption amounts to stating that the ageostrophic wind component $\mathbf{v}_a = \mathbf{v} - \mathbf{v}_g$ depends on λ as

$$\mathbf{v}_a \sim \frac{1}{10} (L/a)f\lambda \quad (21)$$

The Coriolis force of the ageostrophic component at scale λ becomes

$$\{(\mathbf{v} - \mathbf{v}_g) \times \mathbf{k}f\}_\lambda \sim \frac{1}{10} (L/a)f^2 \lambda \quad (22)$$

At $\lambda \sim L$ this term is of order $10^{-4} \text{ msec}^{-2}$, but at $\lambda \sim 0.1 L$ (corresponding to wavelengths of about 400 km) this term is of order $10^{-5} \text{ msec}^{-2}$. Therefore, subgridscale eddies make small contributions to the Coriolis force on the

flow field, and there is no need to represent subgrid-scale Coriolis forces by some kind of model if the grid size is of order 100 km. Formally speaking, this need does not exist anyhow, because the Coriolis force is linear in velocity, and the mean value of subgrid-scale fluctuations is zero by definition.

The advective terms do not possess this feature, since they are nonlinear. Linear estimates of nonlinear effects are tricky; in this context, they involve interactions between eddies of various sizes. The vortex force at scale λ , for example, includes large-scale advection of λ -scale vorticity, λ -scale advection of large-scale vorticity, λ -scale advection of λ -scale vorticity, and many other combinations.

Small-scale (λ -scale) advection of λ -scale vorticity scales as

$$\underline{v}(\lambda) \times \underline{k}\zeta(\lambda) \sim (L/a)^2 f^2 \lambda. \quad (23)$$

At a scale $\lambda = 100$ km (wavelengths of 400 km), this effect is of order $10^{-5} \text{ msec}^{-2}$, which is 10% of the overall vortex force. Therefore, this term may be ignored if no great precision is required.

Small-scale advection of large-scale relative vorticity behaves in the same way as (23):

$$\underline{v}(\lambda) \times \underline{k}\zeta(L) \sim (L/a)^2 f^2 \lambda. \quad (24)$$

This is due to the fact that the vorticity is independent of scale. Evidently, all small-scale advection may be ignored in the formulation of approximate equations of motion.

Problems arise, however, when the large-scale advection of small-scale vorticity is considered. This is estimated as

$$\underline{v}(L) \times \underline{k}\zeta(\lambda) \sim (L/a)^2 f^2 L. \quad (25)$$

This contribution is independent of the size of the λ -scale eddies; it is of order $10^{-4} \text{ msec}^{-2}$ at all scales because the vorticity is independent of scale in the inertial range. Strictly speaking, therefore, the equations of motion should contain a term representing the average subgrid-scale vortex force.

Filtering of high frequencies appears to be a suitable solution of this dilemma. Contributions of the type expressed by equation (25) generate angular velocities at the observation point that are of order $v(L)/\lambda$. For $\lambda = 10^5 \text{ m}$ (100 km) and $v(L) = 10 \text{ msec}^{-1}$, the "frequency" is of order 10^{-4} sec^{-1} , which is one order of magnitude larger than the angular velocity in all eddies (the latter is $\zeta \sim 10^{-5} \text{ sec}^{-1}$). It would seem that careful removal of these higher frequencies would alleviate the problem.

If the same analysis is applied to the other part of the advective term (the dynamic-pressure gradient in the equation of motion), the conclusions

obtained above do not change. Apparently, if large-scale advection of small-scale features can be handled somehow, all other contributions to the rate of change of the flow field decrease with decreasing scale. In other words, the evolution of the flow field is dominated by the evolution of its large-scale features. This means that equations of motion without subgridscale eddy terms may describe the evolution fairly well. It also means that numerical prediction methods do not have to be extremely concerned about the limited spatial resolution of the observational network.

In three-dimensional turbulence, on the other hand, the situation is altogether different. In the inertial subrange of 3D turbulence, the kinetic energy spectrum is proportional to the inverse five-thirds power of the wave number, and the characteristic velocity of an eddy of size λ is estimated as

$$u(\lambda) \sim \epsilon^{1/3} \lambda^{1/3} . \quad (26)$$

The vorticity at scale λ is therefore given by

$$\omega(\lambda) \sim \epsilon^{1/3} \lambda^{-2/3} . \quad (27)$$

Here, the Coriolis force also decreases with decreasing eddy size, though not as rapidly as in the atmospheric counterpart:

$$(\underline{u} \times \underline{k}f)_\lambda \sim f\epsilon^{1/3} \lambda^{1/3} . \quad (28)$$

The vortex force corresponding to λ -scale advection of λ -scale vorticity, however, increases as the scale decreases:

$$\underline{u}(\lambda) \times \underline{\omega}(\lambda) \sim \epsilon^{2/3} \lambda^{-1/3} , \quad (29)$$

and the vortex force corresponding to large-scale advection of λ -scale vorticity increases fairly rapidly with decreasing eddy size:

$$\underline{u}(L) \times \underline{\omega}(\lambda) \sim u(L) \epsilon^{1/3} \lambda^{-2/3} . \quad (30)$$

This latter term can be filtered out however, because at a fixed observation point it generates frequencies that are much larger than $\omega(\lambda)$.

We need not search further, because (29) - a term which cannot be removed by filtering - increases as the scale decreases. This shows that the temporal evolution of 3D turbulence is dominated by its small-scale structure. Terms such as (29) cannot be ignored, because the subgridscale contributions may be larger than the contributions made on the resolvable scales. A statistical approach seems inevitable. If the grid size is λ , the equations of motion have to include the average contribution to the vortex force made by all subgridscale eddies. Fortunately, this averaging process removes the large, rapid fluctuations associated with eddies much smaller than λ , so that the proper estimate is

$$\overline{(\underline{u} \times \underline{\omega})}_\lambda \sim \epsilon^{2/3} \lambda^{-1/3} . \quad (31)$$

The task of finding appropriate models of the various components of (31) is a major issue in turbulence theory; here we will restrict ourselves to a numerical estimate. For $\epsilon \sim 10^{-3} \text{ m}^2 \text{ sec}^{-3}$ and $\lambda = 10^5 \text{ m}$ (numbers we used before), we obtain

$$(\underline{\omega} \times \underline{\omega})_{\lambda} \sim 2 \times 10^{-4} \text{ msec}^{-2}. \quad (32)$$

This is only a factor of two larger than the vortex force at the large-scale end (where $L = 10^6 \text{ m}$ is the eddy size). The time step required in numerical computations, however, becomes fairly small, because it has to be geared to the dynamic time scale ω^{-1} of the λ -scale eddies. For $\lambda = 10^5 \text{ m}$, $\omega \sim 4 \times 10^{-5} \text{ sec}^{-1}$, which is four times as fast as the evolution of the L -scale structure.

In numerical work along these lines (Deardorff, 1970 - present) the grid size is nevertheless taken as small as possible, consistent with the computer facilities available. The reason for this approach is that the modeling (parameterization) of average subgrid-scale contributions becomes easier as the grid size decreases.

6. Vorticity Dynamics

One of the most pronounced differences between 3D-turbulence and quasi-2D atmospheric flows is the magnitude of the vorticity fluctuations. In large-scale atmospheric flows the relative vorticity is of order 10^{-5} sec^{-1} at all scales down to a few hundred kilometers, while in the 3D counterpart the vorticity fluctuations are of order 10 sec^{-1} (for conditions with the same large-scale velocities and the same large-eddy size).

This suggests that the study of the vorticity equation should be worthwhile. For an inertial frame of reference, the vorticity equation is

$$\frac{d\omega_i}{dt} = \omega_j \frac{\partial u_i}{\partial x_j} + v \frac{\partial^2 u_i}{\partial x_j \partial x_j}. \quad (33)$$

In vector notation, this is written as

$$\frac{d\underline{\omega}}{dt} = (\underline{\omega} \cdot \nabla) \underline{u} + \nu \nabla^2 \underline{\omega}. \quad (34)$$

The first term on the right-hand side represents two kinds of effects: (a) turning of the vorticity vector direction caused by shear (off-diagonal components of the velocity gradient), and (b) amplification or attenuation of the vorticity amplitude by streaming motions ("stretching" or "squeezing", respectively).

For our analysis, vortex stretching is the most important of these effects. However, in an exactly two-dimensional flow there is no vortex

stretching at all because ω then is at right angles to the gradient operator (which lies in the plane of the flow). Therefore, we must allow some vertical motion in order to keep the stretching term.

In an approximately 2D flow, the vertical component of ω is by far the largest. If we call that component ζ_a (we are still in an inertial frame of reference), and if we ignore viscous diffusion, (34) may be approximated by

$$\frac{d\zeta_a}{dt} = \zeta_a \frac{\partial w}{\partial z} . \quad (35)$$

In incompressible flow, we have

$$\frac{\partial w}{\partial z} = - \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) = - \nabla_h \cdot \underline{v} , \quad (36)$$

where $\nabla_h \cdot \underline{v}$ is the horizontal divergence of the horizontal wind field. If we substitute (36) into (35), we obtain

$$\frac{d\zeta_a}{dt} = - \zeta_a \nabla_h \cdot \underline{v} . \quad (37)$$

For a rotating system, this equation does not change; one common form is (Haltiner and Martin, p. 350)

$$\frac{d}{dt} (\zeta + f) = - (\zeta + f) \nabla_h \cdot \underline{v} . \quad (38)$$

This states that the absolute vorticity is amplified in regions with horizontal convergence, and that it is reduced in regions with horizontal divergence. Convergence leads to convergence of angular momentum, divergences spreads angular momentum over larger areas. Generally speaking, vortex stretching is not at all pronounced on synoptic scales; in hurricanes and tornadoes, however, vorticity amplification leads to destructive concentrations of vorticity and of kinetic energy.

At levels at which the horizontal divergence generally is small (such as the 500 millibar surface, the "middle" of the atmosphere), equation (38) reduces to

$$\frac{d}{dt} (\zeta + f) = 0 . \quad (39)$$

This states that the absolute vorticity is conserved along fluid trajectories. This equation plays a key role in simple models of atmospheric motion and in short-term prediction schemes. It can be generalized to more realistic models by taking it to describe the evolution of such quantities as the pseudo-potential vorticity (Charney, 1971).

Equation (39) implies that vorticity changes are due solely to advection. Now, the Coriolis parameter f does not depend on time or longitude, but it does change as the latitude (y) varies. In a " β -plane approximation" (which uses $df/dy = \beta$, a constant), e.g. (39) may be written as

$$\frac{\partial \zeta}{\partial t} + (\mathbf{v} \cdot \nabla_h) \zeta = -v\beta \quad (40)$$

At any fixed observation point, the only source of relative vorticity (apart from mere advection) is transport of Coriolis rotation in the latitudinal direction. Therefore, at middle latitudes, the relative vorticity level may be estimated as

$$\zeta \sim \beta L \quad (41)$$

where L is the distance over which transport of angular velocity is effective. If we put

$$\beta = \frac{df}{dy} = \frac{f}{a} \quad (42)$$

where a is the earth's radius, we obtain

$$\zeta \sim \left(\frac{L}{a}\right) f \quad (43)$$

This is the foundation for the estimates we used earlier. Because $L/a = 1/6$ if $L = 1000$ km, the relative vorticity in synoptic flows is nearly an order of magnitude smaller than the absolute vorticity.

Does equation (39) imply that nothing at all happens to the absolute vorticity, except for the obvious advective changes? No; two-dimensional flows are capable of increasing vorticity gradients. For incompressible, two-dimensional flow in an inertial frame of reference, the evolution of $\partial\omega/\partial x_i$ is governed by

$$\frac{d}{dt} \left(\frac{\partial\omega}{\partial x_i} \right) + \frac{\partial u_j}{\partial x_i} \frac{\partial\omega}{\partial x_j} = v \frac{\partial^2}{\partial x_j \partial x_j} \left(\frac{\partial\omega}{\partial x_i} \right) \quad (44)$$

The second term on the left hand side tends to amplify vorticity gradients, much as the stretching term in the vorticity equation tends to amplify vorticity.

Two-dimensional flow conserves vorticity, but it amplifies vorticity gradients. Since the increasing gradients cannot be associated with increasing vorticity, they must be associated with decreasing scales of motion. The net effect of (44) must be that vorticity is carried to smaller scales. This amounts to a spectral flux of vorticity. The average flux must conserve enstrophy (mean square vorticity), so simple similitude suggests that the vorticity at any scale λ smaller than L is independent of scale. This leads to the k^{-3} spectrum and to the scale relations we used in Section 4.

We can be brief about 3D turbulence. Vorticity dynamics in 3D turbulence is covered in Section 3.3 of Tennekes and Lumley; it is completely dominated by vortex stretching (something like complex interactions among tornadoes at all scales), and leads to extremely high enstrophy levels. Atmospheric flows are gentle compared to turbulent flows, because they do not possess a mechanism for the nearly unlimited increase of vorticity fluctuations. This makes it a lot easier to predict the evolution of

synoptic flows than the evolution of their 3D counterparts. Statistical techniques are a necessity in 3D turbulence; fortunately, this is not so for large-scale atmospheric flows.

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IV SRG ON AIR-POLLUTION METEOROLOGY

Part 1

TASK 2

W. J. Moroz

SECOND ANNUAL REPORT

IV. SRG on Air-Pollution Meteorology

TASK 2

1.0 Atmospheric Effects on Particulate Pollutants

The objectives of Task 2 are to:

1. Select and establish operating procedures for instruments capable of providing quantitative values to establish particle number size distributions in the atmosphere;
2. Establish chemical analytical procedures which would permit particle identification in the atmosphere in order to establish mass continuity (including loss or addition by difference) for the atmospheric burden of particles;
3. Collect data establishing particle number size distributions applying to selected chemical species which can be used as tracers in following a cloud of particles from a specific urban source; make observations using aircraft in a spatial grid network (horizontal and vertical) to establish particle characteristics and changes in physical characteristics of the particles during their travel time in the atmosphere;
4. Study the behavior of the size distributions as functions of time, location, underlying terrain and pertinent meteorological variables;
5. Initiate development of a model capable of predicting particle behavior in time and space, relative to the source emission, in

terms of particle-number concentrations and size distributions; field observations, suitably processed, will serve as input for the prediction model.

The rationale underlying the above objectives is that information regarding particle-number concentrations and size distributions in the atmosphere is essential to an understanding of the following fundamental processes:

(a) particle removal mechanisms; e.g., fallout, agglomeration, surface deposition, particle growth by moisture condensation;

(b) effects of absorption and scattering of electro-magnetic radiation, especially with regard to visibility and modification of solar radiation. Number-size distributions of particles, total concentration, shapes, (by inference if particle growth by condensation is significant) indices of refraction and surface states of the individual particles (by inference) all contribute to these effects;

(c) potential health effects due to particles at some distance from the point of generation.

Since information describing number-size distributions of particles in the lowest 3000m of the atmosphere over and downwind from urban areas is scarce at the present time, the data our research team is gathering will constitute valuable information in its own right. Particle agglomeration, breakup, nucleation, diffusion and removal are allied problems to be considered and/or resolved in Task 2.

1.1 The Sampling Program

The effort of the second year has focused heavily on the development of a sampling and analysis system capable of identifying the chemical species of particles collected in microgram quantities. Techniques for size distribution analysis described in the first annual report have been used and have proved to be adequate. The CAES optical particle counter was used to size particles in four size ranges and has a lower size limit of 0.4 microns. An Environment-One Condensation Nuclei Counter (CNC) with a diffusion-denuder provided information on particle concentration and responds to particles 0.003 microns and larger. Precise particle counts and sizes were measured using electron microscope pictures. Grids were placed in a Bendix Model 959 electrostatic precipitator (ESP) and particles equal to and larger than 0.05 microns were sized using optical counting methods. The CNC and the CAES counters are essentially instantaneous point readings and are used to establish the location of the plume and to give general particle size data. Manual counting of the particles collected by the ESP is the primary method of analysis for particle size data. The CAES counter is calibrated using a generated aerosol of polystyrene latex spheres. The Whitby 3000 was used to calibrate and establish counting efficiencies for the Environment-One CNC and the Bendix ESP.

The site selected for field investigation was the area downwind from Pittsburgh. This site was chosen because of proximity but, even more, because it is a steel production center which would be a strong, identifiable particle source. Further, the particles emitted

at this source would contain a high concentration of iron and other specific metals which would serve as chemical tracers for following and identifying the plume from a diffuse urban source.

In the initial stages of the work the particles collected by the Bendix ESP were used for chemical analysis. Gold coated teflon was used as the collection surface to avoid interference from collection surface contaminants. Nitric acid was used as the solvent of the metals and atomic absorption spectroscopy as the analytical technique. Numerous attempts were made to analyze the microgram quantities collected in this way. While initial results were promising, calibration routines indicated the technique yielded erratic data. A new procedure has been selected after a series of experiments described in the section of this report entitled "Chemical Analysis of Particulates."

A routine flight plan has been established to permit intercomparisons between flights. A regular forecasting service is provided by the University Meteorology Department and when the selected meteorological conditions exist, a flight is made in one of several directions from the urban source which minimize the local interferences. Wind speed is specified as 5 to 10 knots blowing constantly from the same direction for a 10 to 12 hour period beginning sometime in the morning hours. These conditions are needed to establish a uniform plume down wind from the urban source. Tight and specific constraints have severely restricted the number of flights which could be made.

In the field program a preliminary survey is conducted immediately preceeding entry into the "flight plan". Passes are made upwind and downwind of the city and using particle detection instrumentation and

wind direction data the position of center line of the plume is estimated. Flight paths are chosen at right angles to the plume center line at 12 1/2 kilometer intervals to 100 kilometers from the source center. Each path is 10 minutes in length, the center line is crossed at approximately the 5 minute mark, and an ESP sample is taken over that 10 minute interval. The instantaneous particle counters show the particle concentration in the plume during the sampling on a given flight path. As time and weather conditions permit, this "flight plan" is repeated at other altitudes within the surface mixing layer.

The aircraft is equipped with instrumentation to record on magnetic tape every second of the time, the coordinates of the location of the aircraft, the altitude, the temperature, the ground temperature, the relative humidity, the wind speed and direction, the readings on the four channels of the CAES particle counter and the CNC reading. Computer programs have been written to reduce and to present these data.

1.2 Chemical analysis of particulate matter

Since erratic results were being obtained using the initial chemical analysis techniques substantial efforts have been directed toward refinement of the sampling and chemical analysis procedures necessary to interpret the very small masses of particles obtained during short sampling periods. This refinement is critical for aircraft sampling at higher altitudes because of the decrease in sample mass relative to a similar ground level sample. Further, it is essential to establish a sampling analysis scheme which will

provide a "blank" (a sampling surface on which no particles have been collected) level which is as low as possible, and at the same time provide for efficient collection of small particles ($d_p > 0.1 \mu\text{m}$) in a form readily amenable to analysis by flameless atomic absorption spectroscopy which provides the analytical precision required.

The initial chemical analysis system tested was a modification of the Varian Techtron Model 63 Carbon Rod Atomizer (CRA). It consisted of a small disc of type MF Millipore filter (MF) which was inserted directly into the CRA Carbon Cup furnace. Five holes were drilled through the bottom of the cup to provide air flow through the MF, and the sample was collected in this unit. Although the system is quite efficient in its sampling ability, it was found to be much less than satisfactory for analysis of certain metals; particularly Fe, Zn, and Mg due to a high level of these metals as an impurity in the filter matrix. Thus, a very high, undesirable concentration of metals in the blank was the result. The problem is compounded by the very sharp "flash point" of the MF when subjected to ashing in the CRA. It was necessary to modify the procedures to meet the requirements of the field sampling program.

The carbon cups are now available commercially in porous form. This porous graphite appeared to be an efficient matrix for trapping particles and was substituted for the MF system described previously. As before, air filtration was quite efficient, and low volume (low mass) samples seemed adequate. However, we observed definite decreases in filtration efficiency upon successive atomizations in the CRA and only one determination could be allowed per cup, substantially increasing

operating costs. It also reduced to one the number of elements which could be determined per sample, and eliminated the possibility of duplicate determinations on any one sample.

It became obvious that a much more desirable filtration-analysis scheme should involve a larger filter assembly which would allow higher volumes of air in shorter time periods to obtain larger sample masses and to make it possible to perform multi-element analysis on single samples. We decided to further study the MF filter because of its efficiency for particle removal. The plan was to sample with a 47mm MF filter, and dissolve the MF and the particles in nitric acid. Experiments using one 47mm disc of MF in 10ml nitric acid (40%) yielded low blanks for Mn, Cu, Co, Ni, and Cr but much higher blanks (contamination) for Fe, Zn, and Mg; three metals of primary interest in the industrial emissions from a steel manufacturing center. The high background in the blank was contributed partly from impurities in Reagent grade nitric acid, as well as contamination in the filter matrix.

Preliminary tests with Nuclepore filters (NF) showed promise with respect to filter stability in strongly acidic solutions. A 5 minute NF soak in concentrated nitric acid showed effective removal of Fe, Mn, Mg, Co, Cu, Cr, Ni, and Zn contaminants which are found in the commercial NF. (Although NF contaminants are present in lower levels than in the MF, the NF contaminants can be removed with acid treatment prior to sampling. This is not possible with the MF.) After sampling, previous experience suggested particles could be removed from the NF using the nitric acid solution. Field sampling was undertaken to test the existing system.

Preliminary samples were taken at the Tussey Mountain fire tower, which is a remote site free of particles from man-made sources simulating upper level atmospheric particle concentrations. The filters used had pore diameters of 0.05 and 0.10 microns. The conclusion from these field experiments was that the individual samples showed poor correlation between sample volumes and weights of metallic impurities detected chemically. With the use of Ultrapure nitric acid (ULTREX, J. T. Baker), significant decreases in blank levels were observed for Mg, Cu, Al, Mn, Cr, Zn, and Fe and further sampling at the Tussey Mountain Site was undertaken. Filter cleaning procedures have been modified (use aqua regia as particle solute and ultrasonic cleaning of filters to assure all particles are removed from filters) further on the basis of field experience.

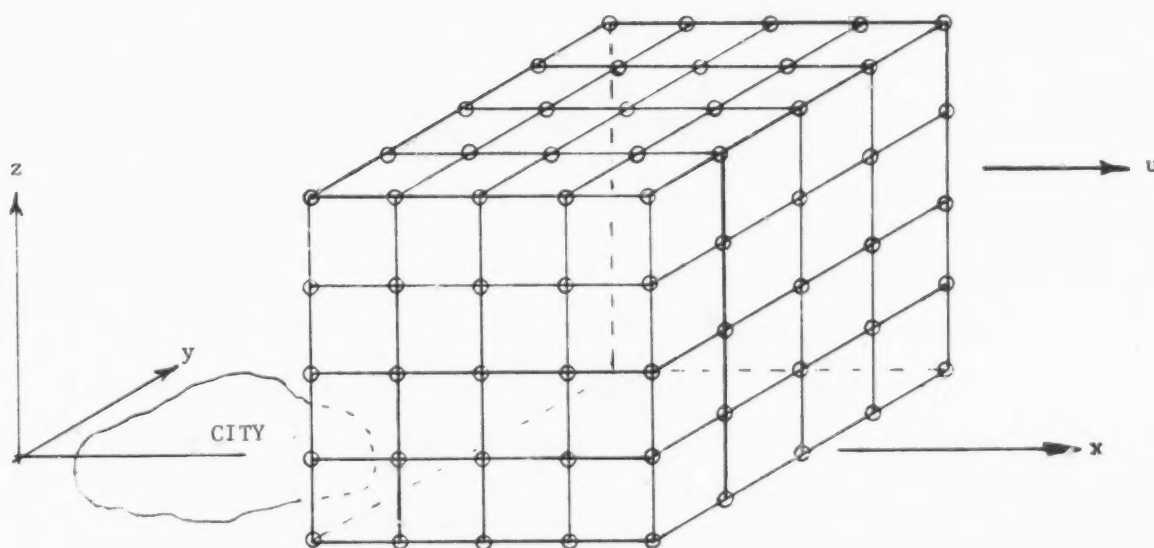
In summary, the development of this method for low-volume sampling of particulates is in the final stage. An optimum filter medium (Nuclepore filters) which is amenable to a necessary chemical decontamination step prior to sampling has been chosen and we have found a suitable means for processing these particulate samples into a solution form which is readily analyzed with high sensitivity using flameless atomic absorption spectroscopy.

1.3 The Numerical Modeling Program

The objective of this aspect of the task 2 is to develop numerical methods which will allow the prediction of changes in particle concentration on a size distribution basis, as the air containing particles

travels downstream from the particle source. A mesoscale model of dimensions comparable to the width of a large city or travel distances between two large cities (about 100 km) is postulated.

The configuration of the model is shown in the following figure.



The concentration distribution of particles on the grid points at the first cross section downstream from the city is assumed to be Gaussian and is computed from the following equation.

$$n(r,t) = \frac{Q(r,t)}{2\pi \sigma_y \sigma_z \bar{u}} \left[\exp \left[\left\{ -\frac{(y-y_s)^2}{2\sigma_y^2} \right\} + \left\{ -\frac{(z-z_s)^2}{2\sigma_z^2} \right\} \right] \right. \\ \left. + \exp \left[\left\{ -\frac{(y+y_s)^2}{2\sigma_y^2} \right\} + \left\{ -\frac{(z+z_s)^2}{2\sigma_z^2} \right\} \right] \right]$$

where $n(r, t)$ is the number concentration of the particles of radius r , $Q(r, t)$ is the total source strength for particles of radius r , y_s and z_s are the co-ordinates of the source and the rest of the symbols are conventional.

The particle concentrations at the grid points are calculated using a finite difference form of the particle diffusion equation.

$$\frac{\partial n(r, t)}{\partial t} + u_j \frac{\partial n}{\partial x_j} = -v_s \frac{\partial n}{\partial x_s} + \overline{K}_j \frac{\partial^2 n}{\partial x_j^2} + C$$

where u_1 , u_2 and u_3 are the conventional three dimensional velocities u , v and w and x_1 , x_2 and x_3 are x , y and z respectively.

v_s is the Stokes fall velocity for particles with a Cunningham correction factor and molecular "slip" factor applied as appropriate for small particles. (See Fuchs, p27.)

$\overline{K}_x$ is an atmospheric diffusivity which is calculated as a function of atmospheric variables. (As in Sheih and Moroz, 1973.)

and C is a coagulation term following Friedlander (1960).

A program for this model has been written and is currently being "debugged." Dr. Sheih is continuing to work with us on development of this model despite his transfer to Argonne National Laboratories because of his personal interest in the activity.

1.4 Progress in Field Sampling of Agglomeration

A total of twenty field trips have been made in addition to the three reported in the first annual report. Thirteen ground level operations and seven aircraft flights were conducted. Of the flights, five were made in St. Louis in connection with the RAPS program in August 1973 and two flights were centered around the Pittsburgh urban area in January and February of 1974.

For the most part the ground level trips were designed for instrument check out and for gathering samples to perfect the chemical analysis techniques. As was noted in the section on chemical analysis, this has been a difficult and time consuming part of this work.

Aircraft sampling has been delayed by unsuitable meteorological conditions and by the availability of the airplane. In order to observe the behavior of particles downstream from an urban complex it is necessary to have persistent meteorological conditions and a minimum of interference from terrain and from particulate input from other sources. Analysis of data obtained during the St. Louis flights indicated that the wind was light and variable during field experiments. The plume downwind of that urban area was not well defined. Results from flights in the Pittsburgh area indicated that interference from terrain and other major sources in the area resulted in distorted interpretations. Analysis of the data did provide preliminary information which are presented as tentative.

Table I shows particle number and mean diameter (corrected to sea level) obtained using the Rich 100 CNC. Particle concentrations do decrease as one moves away from the center city and as the altitude increases from 2600 to 6600 ft. above sea level, as expected. The mean diameter readings are not sufficiently precise to be truly meaningful but are presented as a matter of interest.

TABLE I

Particle Concentrations (Particles/cc) and Mean Diameters (Microns) Downstream from St. Louis at Three Levels Calculated from Rich 100 Condensation Nuclei Counter (Flight 103, August 17, 1973). All observations are below the top of the base layer.

		Downstream Position (km) in Direction of Mean Wind				
		Upstream	25	50	75	100
A. Level 1500 MSL						
Particle Conc.		34,600	14,000	14,600	5,900	3,900
Mean Diameter		0.008	0.0085	0.014	0.006	—
B. Level 2600 MSL						
Particle Conc.		450	16,400	14,100	6,500	5,100
Mean Diameter		0.007	0.005	0.014	0.009	0.014
C. Level 6600 MSL						
Particle Conc.		340	7,100	6,800	950	2,300
Mean Diameter		0.01	0.0045	0.005	0.013	0.0075

After looking at the data in a number of ways, it was determined that plots of $dS/d(\log D)$, where S is particle surface area calculated assuming spherical particles and D is particle diameter, were most sensitive to small changes in particle number and characteristics. In this type of presentation the area under the curve is proportional to the surface area in a given size range and an aerosol containing larger particles will have a smaller total particle surface area than an aerosol containing the same mass of smaller particles. Data from St. Louis flights 103 and 105 are presented in Figures 1 through 6. Figures 1, 2 and 3 are from flight 103 and represent samples collected at three altitudes. The distributions were obtained using the Bendix electrostatic precipitator. The distributions are generally bi-modal or tri-modal. In all three figures there is a shift in the diameter corresponding to the peak concentration as one moves away from the center of the city and at the same time there is a decrease in the area under the curve. Comparing Figures 1 to 2 and 2 to 3 one notes that as the altitude increases the distributions at various distances from the source become more alike. These same observations hold for Figures 3 through 6 which present a similar set of data from Flight 105. Unfortunately the Pittsburgh flight labeled 102 was made at only one altitude. Figure 7 is the data presentation for that flight. Again the same trends appear as in the other two data sets.

Tentatively, the following conclusions may be drawn from these data:

1. As one moves away from the urban center, the maximum concentration of particles in a given size range decreases. At the same

time the size for which maximum concentration occurs shifts to larger particles indicating significant agglomeration. This effect is contrary to that which would be expected if only particle removal by fallout is considered.

2. As one moves away from the earth's surface the particle surface area analysis shows a shift toward uniformity. This may suggest that as agglomeration proceeds, the fall velocity of particles becomes significant in determining the particle distribution in the atmosphere; that is, larger agglomerated particles with higher fall velocities are not diffusing to upper levels.

Gaussian diffusion models may yield incorrect concentrations at both upper and lower levels if these tentative results are further confirmed.

It was determined after the analysis of the Pittsburgh data that the terrain and strong, outlying particle sources in the area surrounding this urban center introduced variables which made analysis very difficult and reduced confidence in conclusions. Recognizing that a relatively flat area with no outlying particle sources is most desirable for field studies we are considering other experimental sites. Currently we are trying to obtain permission from the Canadian Government to fly in the Hamilton, Ontario region. Hamilton has a large steel complex so all currently developed techniques are fully applicable; it is located on Lake Ontario and is situated so that prevailing winds from the west and southwest carry the plume over the lake. It is within easy flying distance and offers the same advantages, with respect to logistics, which Pittsburgh has. Alternatives to Hamilton are Buffalo and New York City.

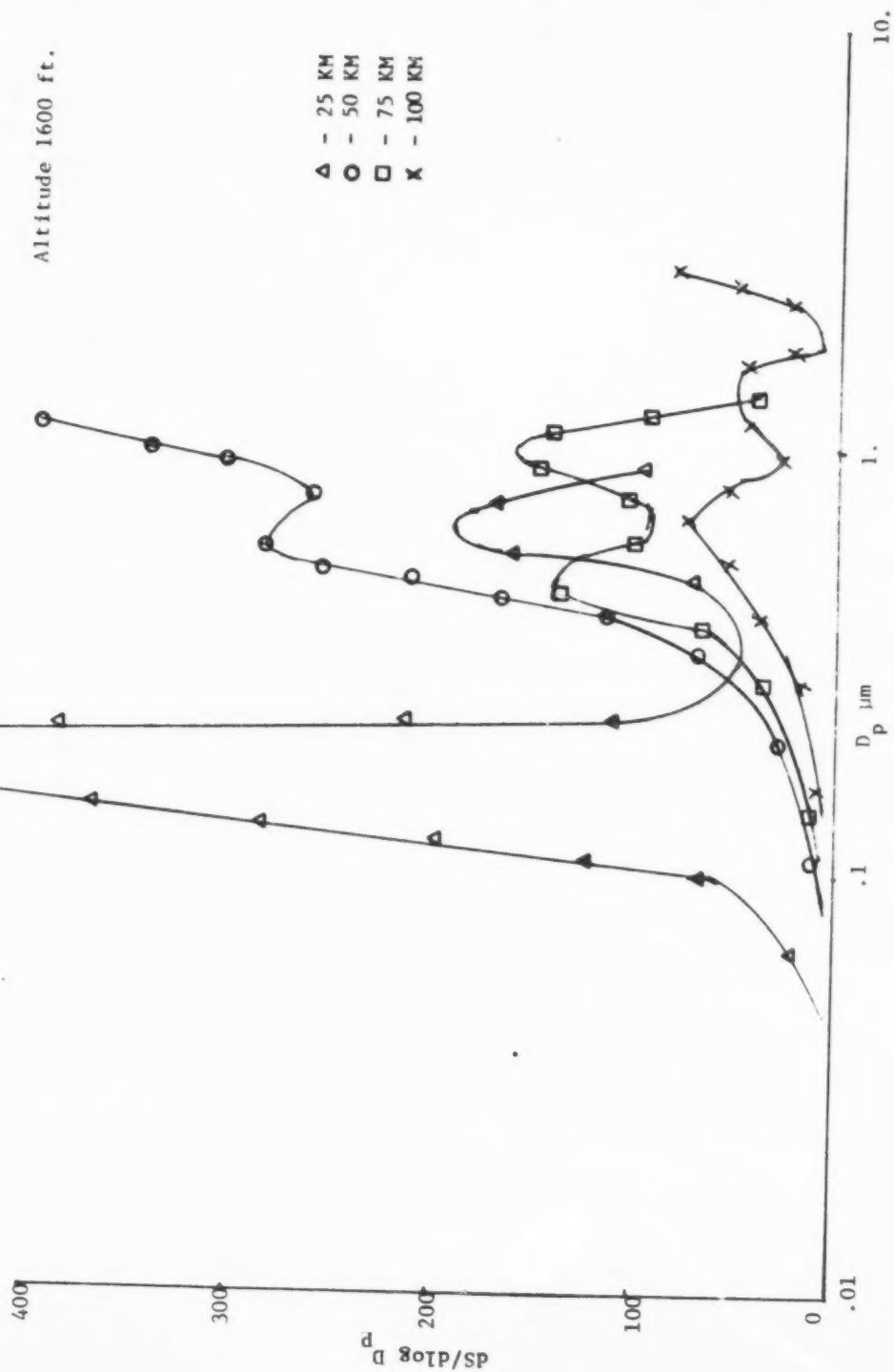
References

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- Sheih, C. M. and W. J. Moroz, 1973; "A Lagrangian Puff Diffusion Model for the Prediction of Pollutant Concentrations over Urban Areas", Proc. 3rd Int. Clean Air Congress, Düsseldorf.
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DS/DLOGD

St. Louis 103 August 1973

Altitude 1600 ft.



DS/DLOGD

St. Louis 103 August 1973

Altitude 2600 ft.

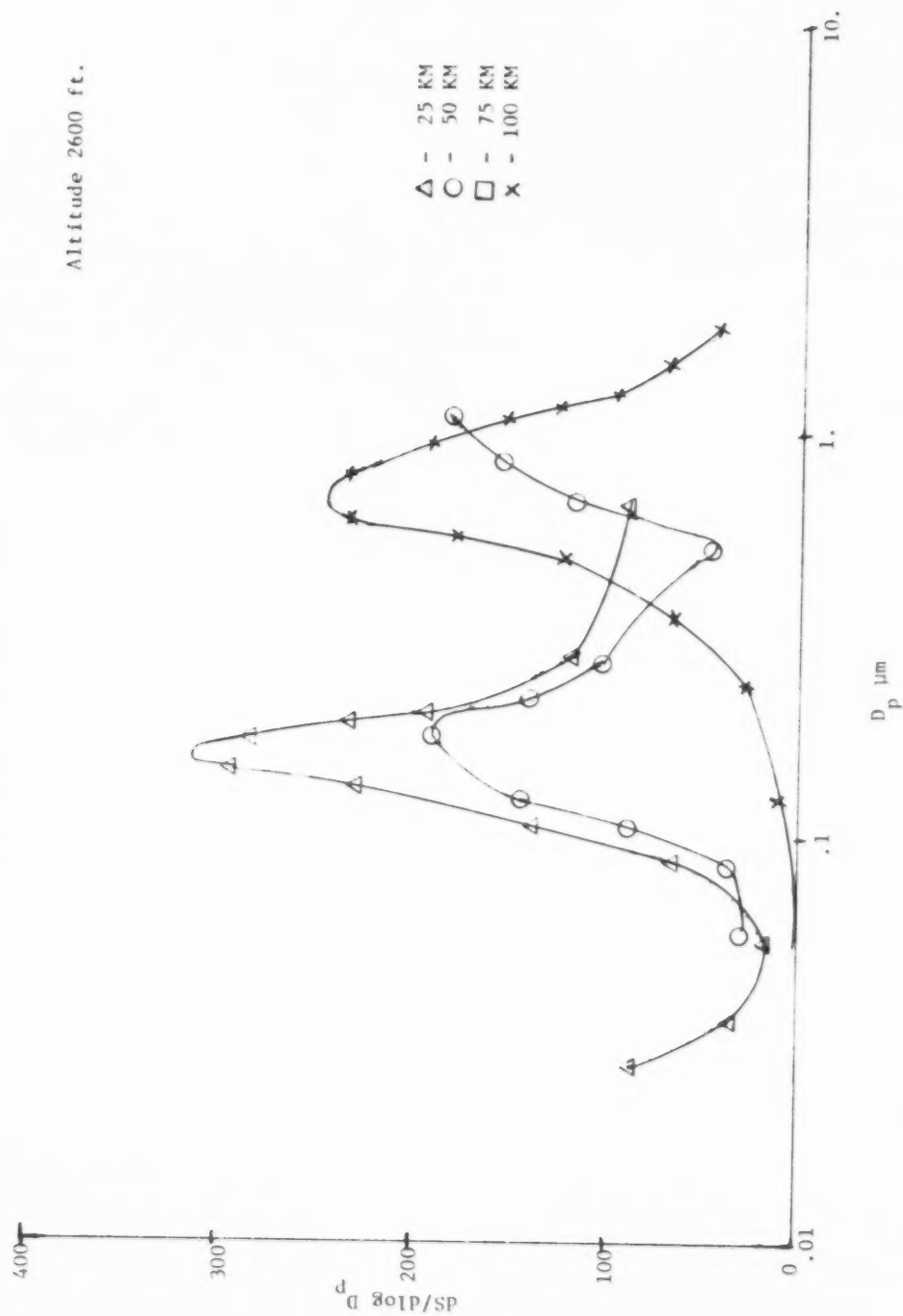


Figure 2

DS/DLOG D
St. Louis 103 August 1973

Altitude 6600 ft.

△ - 25 KM
○ - 50 KM
□ - 75 KM
x - 100 KM

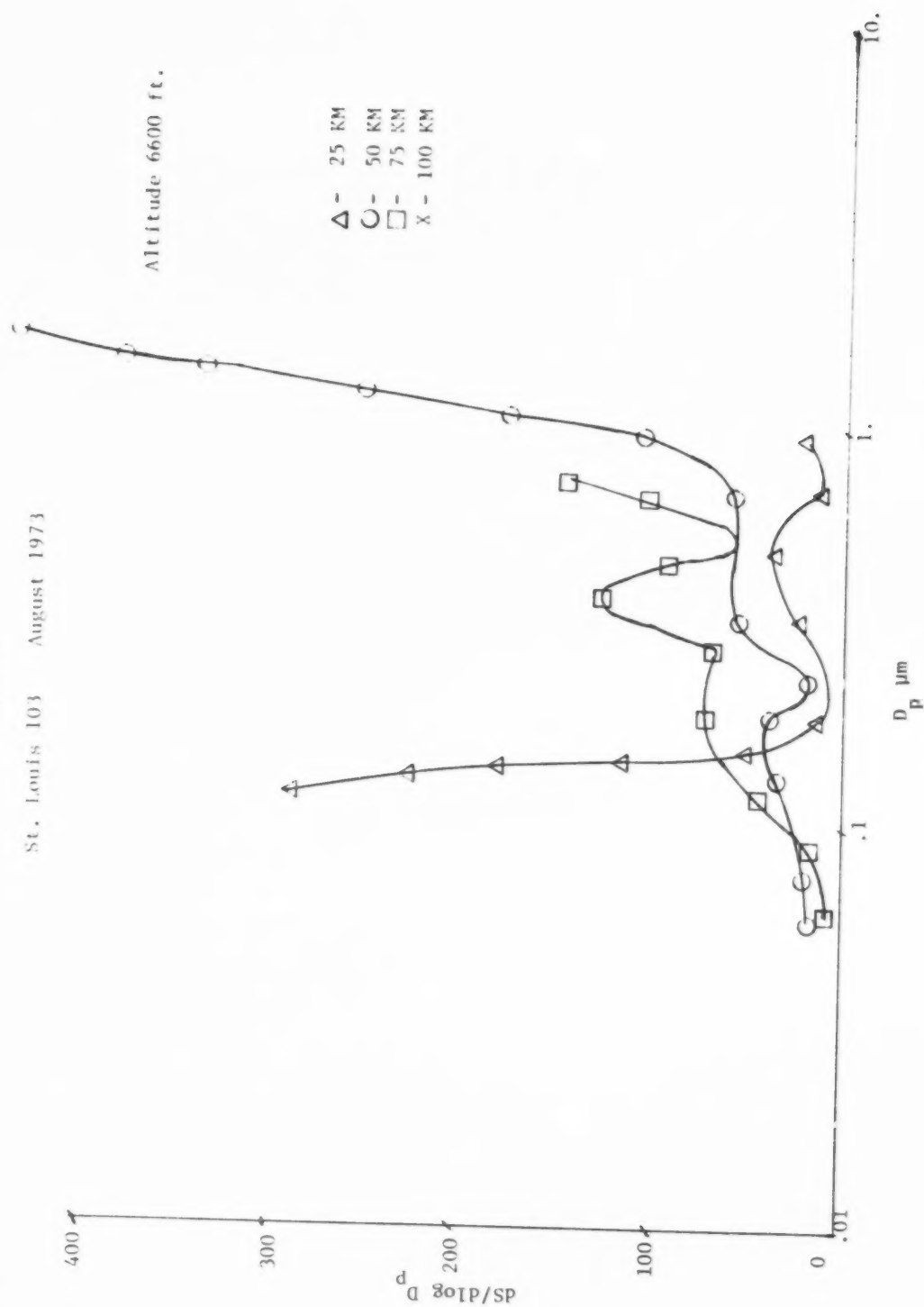


Figure 3

DS/DLOG D

St. Louis 105 August 1973

Altitude 1700 ft.

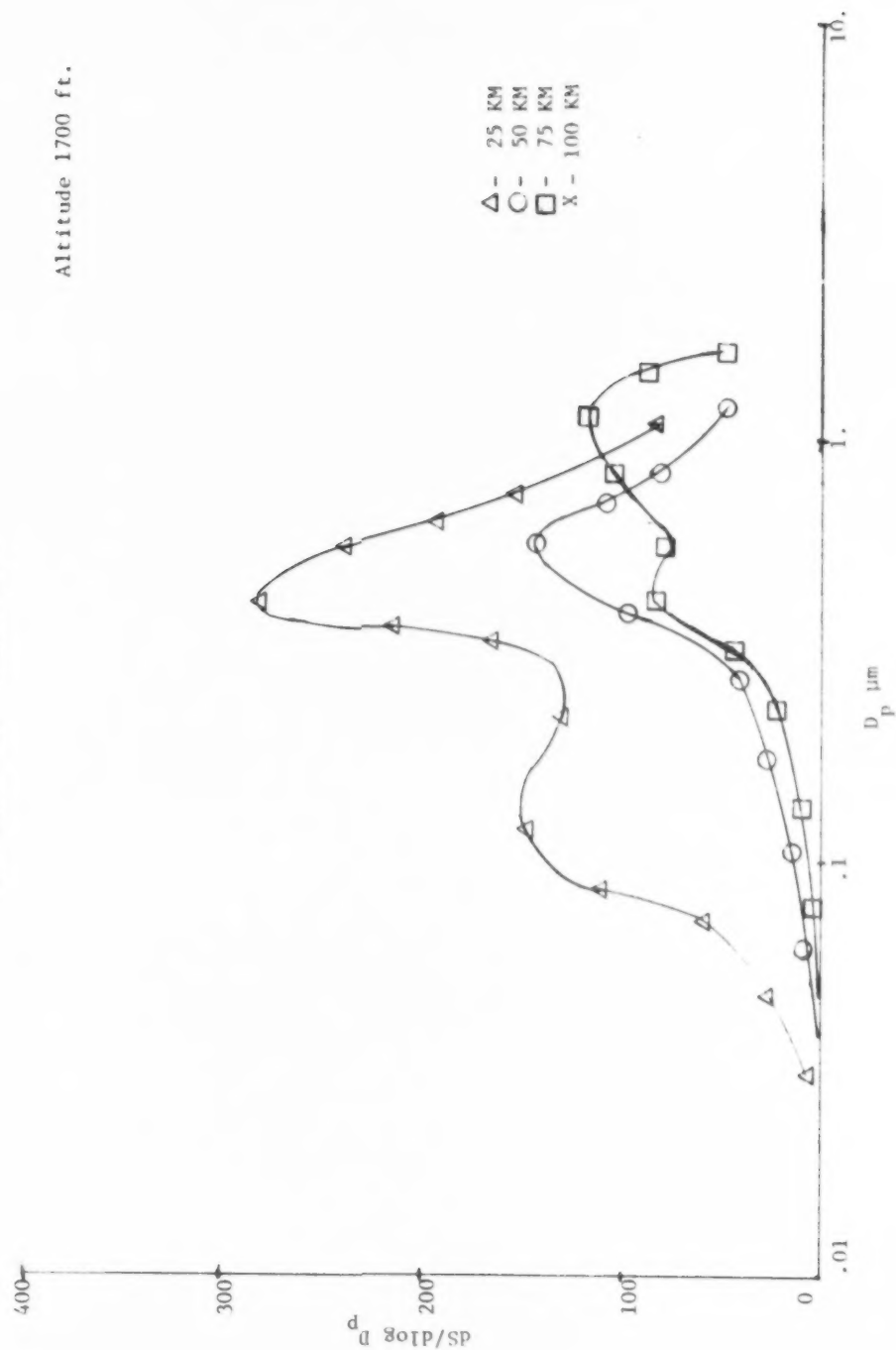
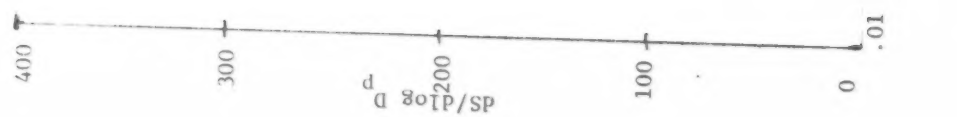


Figure 4

DS/DLOG D

St. Louis 105 August 1973

Altitude 3200 ft.



Δ - 25 KM
 $\circ$ - 50 KM
 $\square$ - 75 KM
 $\times$ - 100 KM

Figure 5

DS/DLOGD

St. Louis 105 August 1973

Altitude 5000 ft.

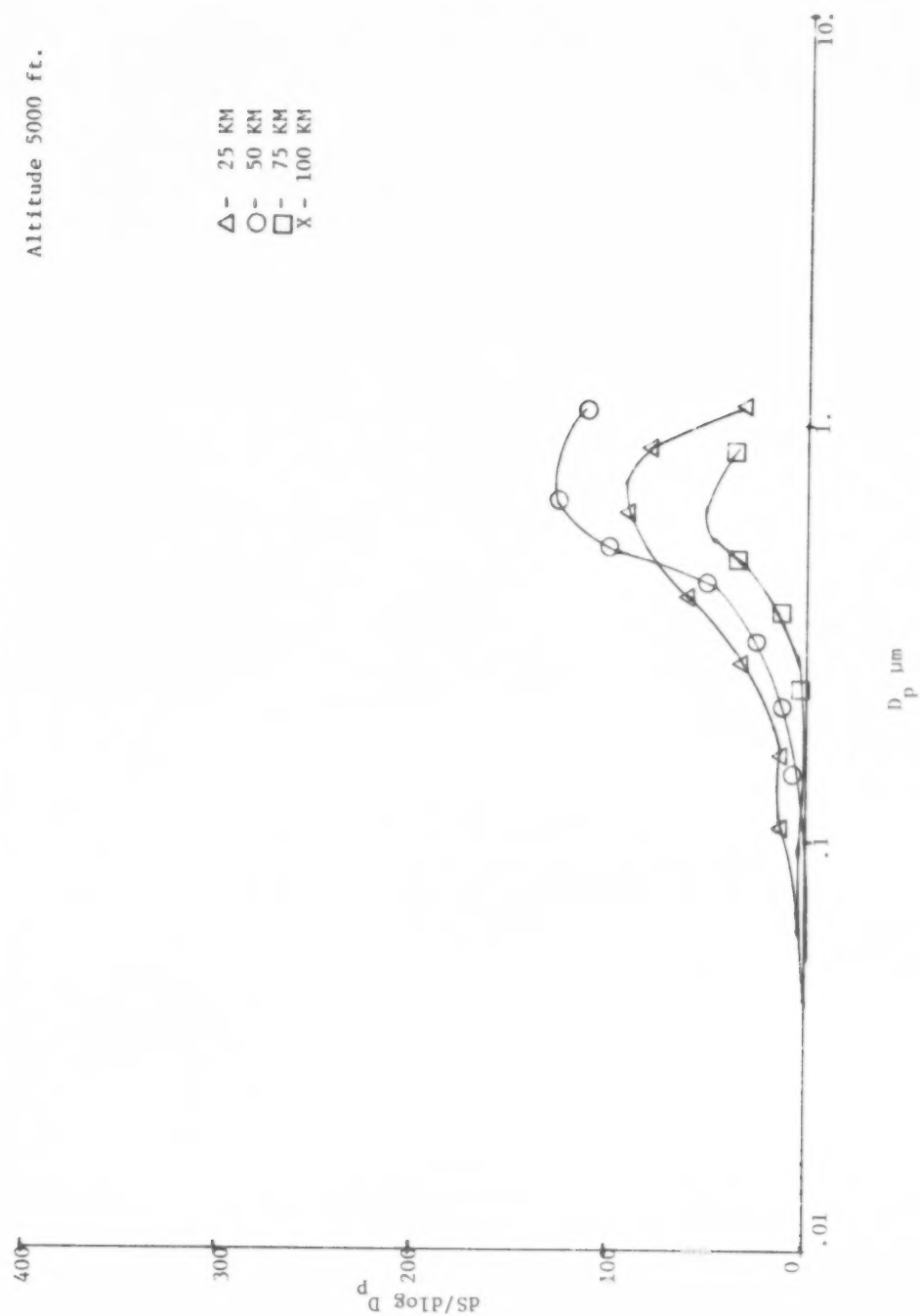


Figure 6

DS/DLOGD

Pittsburgh 102 February 1974

Altitude 3500 ft.

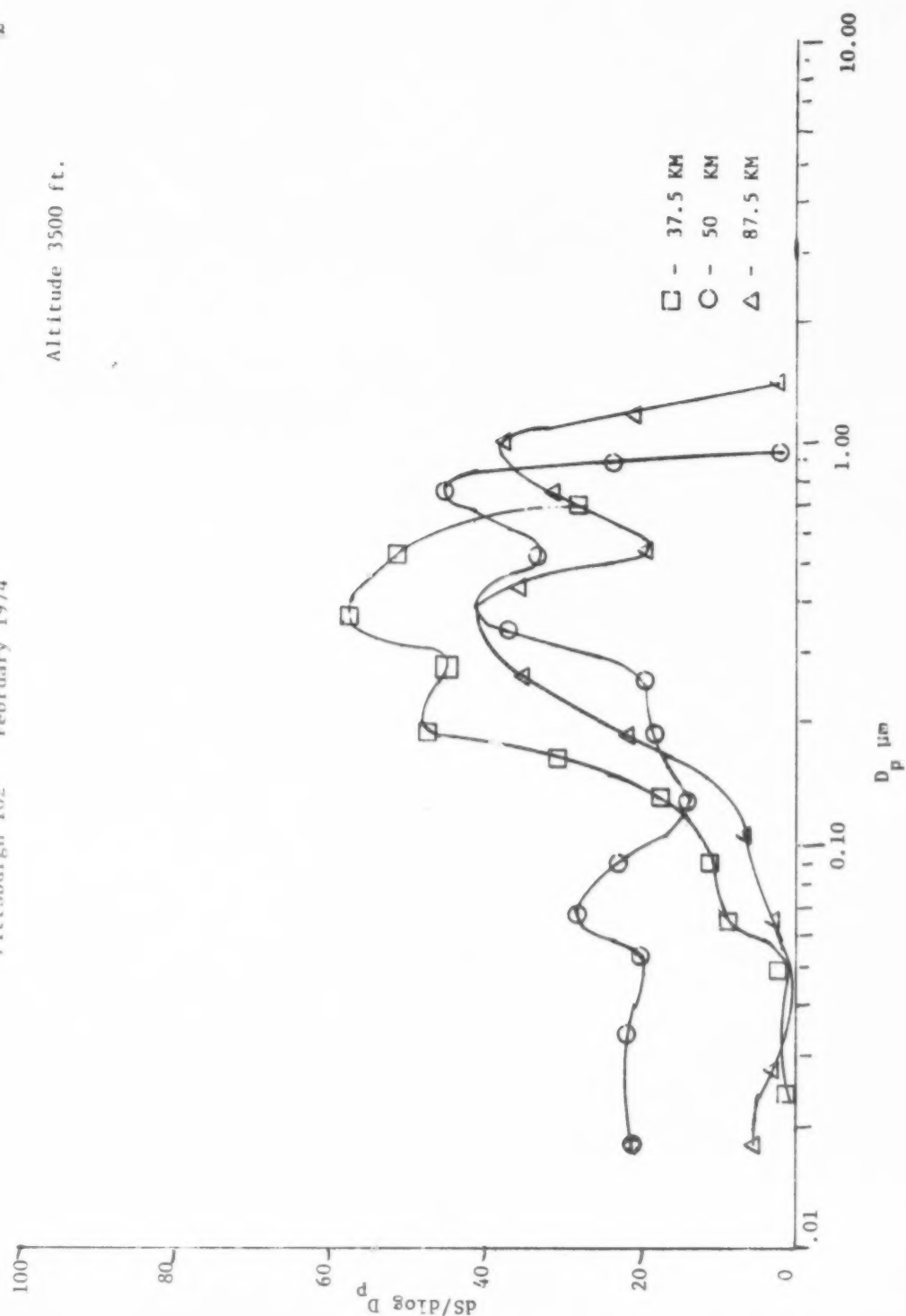


Figure 7

IV ATMOSPHERIC REMOVAL PROCESSES FOR AIR POLLUTANTS

Part 2

TASK 3

R. L. KABEL

IV. Atmospheric Removal Processes for Air Pollutants
Part 2
Task 3

R. L. Kabel

This first portion of the Task 3 annual report presents the intended timetable for the anticipated five year project duration. Brief status statements are included at this point. Extended discussion of accomplishments follow.

1.1 Synopsis

The first year and a half were devoted to a literature review in which potential natural processes for pollutant removal were identified. Background levels as well as natural and man-made sources were also included for perspective. The relevant data on rates of removal by the various mechanisms were assembled. The few quantitative models were scrutinized. The results of the survey are an EPA Grant Report (Rasmussen, Taheri, and Kabel, 1974) and a much abbreviated version of the full report which has been accepted for publication in Water, Air and Soil Pollution. Since the lengthy report is already in the hands of the EPA, the paper is included here as an indication of the work in the first phase of Task 3.

The second and third years are planned for preliminary modeling. Very few documented quantitative data are available in the literature for natural modes of pollutant removal. Still fewer mathematical models exist with demonstrated predictive or even correlative capability. Work is already underway in this area as illustrated later in this report.

Experimental work in the field or laboratory may be taken up in the third and fourth years as appropriate. It is expected that information available in the literature will be inadequate for the development of reliable models. Information gaps will have to be filled or tolerated. The Task 3 budget for experimental work will suffice for no more than a few brief, simple laboratory investigations. Only limited planning has occurred so far in this area. A research proposal to seek funding for such work is in the very first draft stage.

In the fourth and fifth years refined modeling and integration of these models into the comprehensive SRG air pollution-meteorology model are anticipated. The only step taken toward this goal is the decision to focus on sulfur dioxide. The bases for this decision are:

- 1) the importance of SO_2 as a pollutant,
- 2) the consequent greater extensiveness of data and understanding available for SO_2 and
- 3) the fact that SO_2 exhibits more of the various removal mechanisms to a significant extent than do most other pollutants.

1.2 Personnel

With the completion of the first phase of Task 3, the task force has been altered somewhat corresponding to the shift in emphasis toward quantitative modeling. The task leader is Dr. R. L. Kabel, a chemical engineer with interests in reaction kinetics, adsorption, transport phenomena, and mathematical modeling of naturally occurring processes. Continuing are faculty consultants Dr. D. D. Davis, a plant pathologist active in pollutant - vegetation interactions,

and Dr. R. G. de Pena, a meteorologist with interests in atmospheric chemistry and pollutant washout by rain or snow. Also continuing is Mr. L. B. Hausheer, a chemical engineering graduate student. Leaving the task force are Dr. F. E. Wickman, a geochemist who has returned to his home in Sweden; Dr. M. Taheri, who has completed his sabbatical leave from Pahlavi University in Iran; and Miss K. H. Rasmussen, who has completed the requirements for the degree of Master of Science in Geochemistry. Joining the team this fall is Mr. R. A. O'Dell, a graduate of Rensselaer Polytechnic Institute in Environmental Engineering. Mr. O'Dell is supported by an Air Pollution Traineeship through the Center for Air Environment Studies and seeks a Master of Science degree in Environmental Pollution Control.

1.3 Accomplishments

1.3.1. The literature survey phase phase is covered by the following paper which will appear in Water, Air, and Soil Pollution, an international journal of environmental pollution.

GLOBAL EMISSIONS AND NATURAL PROCESSES
FOR REMOVAL OF GASEOUS POLLUTANTS

by

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ABSTRACT

This review attempts to briefly illustrate what the "state of the art" is in the recognition of the various sources and natural sinks of gaseous pollutants. The removal mechanisms include absorption by vegetation, soil, stone, and water bodies, precipitation scavenging, and chemical reactions within the atmosphere. The nature and magnitude of anthropogenic and natural emissions of the gases discussed (H_2S , SO_2 , N_2O , NO , NO_2 , NH_3 , CO , O_3 , and hydrocarbons), along with their ambient background concentrations and information on their major sinks identified to date, are discussed.

INTRODUCTION

The last decade has witnessed an unprecedented interest and concern in the development of mathematical models for predicting air pollutant concentrations. The aim of such models is to define the complicated relationship between air quality and emission rates. The interest in air pollution modeling is based on its potential value in nearly all practical problems involving quantitative consideration of air quality relative to the source location and emission rates. These include the forecasting of undesirable levels of pollution, abatement strategies, long range air resource management programs and urban planning.

Because of energy shortages and use of lower quality fuels it is now more urgent that we develop a much better ability to forecast the consequences of increased pollutant emission. While considerable effort has been devoted to characterizing emissions from anthropogenic sources and their turbulent transport and convection, very little has been done to determine the extent of emission from natural sources and to characterize the processes that clean the atmosphere. Therefore, for a more realistic air pollution model, it is necessary to quantify natural emissions and removal mechanisms. The purpose of this study is to provide quantitative information on source and removal mechanisms so that a realistic air pollution model can be constructed.

Pollutants may be emitted to the atmosphere from many diffuse natural and anthropogenic sources. The natural sources of many gases as shown in Table I far exceed the anthropogenic sources on a global basis. However, because such gases are usually well distributed throughout the atmosphere their concentration, known as the background concentration,

is extremely low. Anthropogenic sources of many pollutants are centered near urban complexes and therefore, their local pollutant concentrations are high and pose a major threat to the urban environment.

The removal of air contaminants from the atmosphere can take place by various mechanisms. A review of these mechanisms and their significance was given by Robinson and Robbins (1968) and more recently by Hidy (1973). The important mechanisms are:

- (1) precipitation scavenging in which the pollutant is removed via two modes. The first is termed "rainout" which involves absorption of gases in the cloud. The second is called "washout" which involves both absorption and particle capture by falling raindrops;
- (2) chemical reactions in the atmosphere including the stratosphere which produce either aerosols or oxidized products such as carbon dioxide and water vapor;
- (3) dry deposition which involves absorption by aerosols and subsequent deposition on the earth's surface; and
- (4) absorption by various substances at the earth's surface including vegetation, soil, stone, and water bodies.

This report presents an analysis of various sources and natural removal processes which should be reflected in the results obtained by air pollution mathematical modeling. Consideration of natural sources and more importantly removal processes in the mathematical modeling not only will yield more accurate results, but will provide a basis for determining the possibilities of expanding local air pollution models to regional or global scales. This study has considered various pollu-

tants including sulfurous compounds, nitrogenous compounds, carbon monoxide, ozone, and hydrocarbons. The analysis is presented in a similar form for each compound including data on ambient concentrations, sources, and mechanisms of removal. An overview of this paper is provided by Table I.

The quantitative information given in this paper has, in most instances, been subject to conversion of units. The conversions were made to attain some consistency among the data and with the International System (SI) of Units.

Table I. SUMMARY OF SOURCES, ANNUAL EMISSION, BACKGROUND CONCENTRATION AND MAJOR SINKS OF ATMOSPHERIC GASEOUS POLLUTANTS

Pollutant	Major Source		Estimated Emission, Kilogram	Background Concentration $\mu\text{g}/\text{m}^3$	Major Identified Sinks
	Anthropogenic	Natural	Anthropogenic	Natural	
SO_2	Combustion of coal and oil	Volcanoes	130×10^9	2×10^9	1-4 Scavenging; Chemical reactions; Soil and surface water absorption; Dry deposition
H_2S	Chemical processes; Sewage treatment	Volcanoes; Biological decay	3×10^9	100×10^9	Oxidation to SO_2
N_2O	None	Biological decay	None	590×10^9	Photodissociation in stratosphere; Surface water and soil absorption
NO	Combustion	Bacterial action in soil; Photodissociation of N_2O and NO_2	53×10^9 combined with NO_2	768×10^9	Oxidation to NO_2
NO_2	Combustion	Bacterial action in soil; Oxidation of NO	4×10^9	170×10^9	Photochemical reactions; Oxidation to nitrate; Scavenging
NH_3	Coal burning; Fertilizer; Waste treatment	Biological decay	360×10^9	3000×10^9 (7)	Reaction with SO_2 ; Oxidation to nitrate; Scavenging
CO	Auto exhaust and other combustion processes	Oxidation of methane; photodissociation of CO_2 ; Forest fires; Oceans	70×10^9	300×10^9	Soil absorption; Chemical oxidation
O_3	None	Tropospheric reactions and transport from stratosphere	-	(7)	Photochemical reactions; Absorption by land surfaces (soil and vegetation); Surface water
Non-Reactive hydrocarbons	Auto exhaust; Combustion of oil	Biological processes in swamps	27×10^9	175×10^9	Biological action
Reactive hydrocarbons	Auto exhaust; Combustion of oil	Biological processes in forests	27×10^9	175×10^9	Photochemical oxidation

SULFUR CONTAINING GASES

The two primary sulfur containing gases present in the atmosphere are hydrogen sulfide (H_2S) and sulfur dioxide (SO_2). Hydrogen sulfide, the most reduced form of sulfur, is not considered to be an air pollutant per se, for its primary modes of origin are natural processes. Its importance arises from the nature of the chemical reaction it is subject to once it has been released to the atmosphere. That reaction is its rapid oxidation to sulfur dioxide. As such, H_2S has often been thought of as a "natural" source of SO_2 .

Accurate measurements of the background concentration of hydrogen sulfide in the atmosphere are not as yet available. Measurements over Bedford, Massachusetts, and New York City performed by Junge (1963) found values ranging from $2\text{--}20\text{ }\mu\text{g}/\text{m}^3$ ($1.4\text{--}14\text{ ppb}$). Robinson and Robbins (1968) estimate H_2S concentrations in clean air to average $0.3\text{ }\mu\text{g}/\text{m}^3$ (0.2 ppb). The National Center for Atmospheric Research (NCAR) (as cited in Kellogg et al., 1972) has shown these measurements to be unreliable because they were made using liquid scrubbers. These scrubbers are faulty in that they allow both the oxidation and loss of significant quantities of H_2S .

Because of early recognition of sulfur dioxide as a primary pollutant capable of inflicting severe illness or even death on humans, extensive research has increased our knowledge of the sources and sinks of this gas far more than any other pollutant. Background concentrations of sulfur dioxide seem to range between $1\text{ and }4\text{ }\mu\text{g}/\text{m}^3$ ($.4\text{--}1.5\text{ ppb}$). Georgii (1970) found concentrations over the Atlantic Ocean ranging from $1\text{--}4\text{ }\mu\text{g}/\text{m}^3$, and over Colorado from $0.5\text{--}2.0\text{ }\mu\text{g}/\text{m}^3$ ($.2\text{--}.8\text{ ppb}$). Cadle et al. (1968) found values over Antarctica ranging from $<1.0\text{ to }3.2\text{ }\mu\text{g}/\text{m}^3$ ($<.4\text{--}1.2\text{ ppb}$).

HYDROGEN SULFIDE

Sources

The primary source of H_2S is decaying vegetation in swamps, bogs, and other land areas. Very little is known about annual rates of H_2S from these regions though, and up to this time estimates that have been made are only the result of balancing suggested sulfur budgets. Estimates of this H_2S source strength range from 58×10^9 kg/yr (Friend, 1973) to 112×10^9 kg/yr (Eriksson, 1960).

The oceans have been suggested as an additional source of sulfides to the atmosphere (Eriksson, 1960). Measurements though have not been conclusive and so estimates on the magnitude of this flux [see Table IV] have been made by determining the value needed to balance a particular portion of the sulfur cycle and equating that value with the flux of $\text{S}^{=}$ from the oceans to the atmosphere. H_2S is also released by volcanoes but the quantity is far less than the amount of SO_2 released. Only relatively minor amounts of H_2S are released from anthropogenic sources.

Removal Mechanisms

Hydrogen sulfide is relatively insoluble in water; at 20°C and 1 atmosphere, the solubility is only 0.385g/100g H_2O . It therefore will not be readily absorbed by vegetation or bodies of water, nor will it be involved in liquid state reactions in the atmosphere. In fact, the only real mode of "removal" is the oxidation reactions it so readily becomes involved in.

H_2S can be oxidized by ozone (O_3), molecular oxygen (O_2) or atomic oxygen (O). Cadle and Ledford (1966) have shown that although the oxidation of H_2S by ozone proceeds quite slowly in a gaseous atmosphere, the reaction is catalyzed by the presence of aerosols. Hales et al.

(1969) have given a rate equation for the change in SO_2 concentration with time as a function of the concentration of both H_2S and ozone.

Oxidation of H_2S by atomic oxygen will probably be significant only in photochemical smog and the stratosphere; the reason being that only in these environments are significant quantities of atomic oxygen available due to the photolysis of ozone. The reaction to proceed first would be:



This is then followed by a reaction chain producing SO_2 , SO_3 , and sulfuric acid (Liuti et al., 1966). As a result of its rapid oxidation, H_2S has a very short residence time in the atmosphere, probably about 2 days (Hidy, 1973).

SULFUR DIOXIDE

Sources

Industrial growth has caused a significant increase in the production and ultimate release of sulfur dioxide to the atmosphere. Robinson and Robbins (1968) estimated anthropogenic activity as the source of 146×10^9 kg SO_2 each year. A study on anthropogenic SO_2 production by the Study of Critical Environmental Problems (SCEP) (M.I.T., 1970) concluded that globally 93×10^9 kg SO_2 were produced in the year 1967-1968. Kellogg et al. (1972) point out that this estimate may be low because the "emission factor" used for this global estimate is probably applicable only in the United States and will be higher in other nations which rely more heavily on fossil fuels with high sulfur contents such as coal. Kellogg et al. believe an estimate of about 100×10^9 kg SO_2 per year would be much more reasonable; of this, almost 94% is emitted in the Northern Hemisphere alone. Friend (1973) has estimated anthropogenic

emissions of SO_2 at 130×10^9 kg per year.

There are, of course, natural sources of sulfur dioxide as well but the total amounts derived from these sources are extremely difficult to quantify. It is believed that most natural SO_2 is released by volcanoes. Kellogg et al. estimate that the quantity released by volcanoes is about two orders of magnitude less than the amount they estimated to be a result of man's activities (1.5×10^9 kg/yr vs. 1.0×10^{11} kg/yr). There is, as the authors point out, a good deal of uncertainty in their estimate. Stoiber and Jepsen (1973) estimated annual volcanic emissions of SO_2 to be 15×10^9 kg, an order of magnitude greater than the estimate of Kellogg et al.

There are no other widely accepted natural SO_2 sources. Kellogg et al. have pointed out that despite the fact that SO_2 is so very soluble in water, sea water might be a source rather than a sink if the right physicochemical conditions prevail. Without further convincing evidence on this subject, one should probably contend that sea water would, in toto, provide only relative minor amounts of SO_2 to the atmosphere, if any at all.

Removal Mechanisms

Sulfur dioxide is very soluble in water; at 20°C and 1 atmosphere the solubility is 10.8 g/100 g H_2O . It is also very chemically reactive and either oxidizes to sulfate or photochemically reacts with other atmospheric contaminants. Therefore, sulfur dioxide is removed from the atmosphere by various mechanisms involving water or other compounds. The major identified sinks for this gas are: precipitation scavenging, chemical conversion, and absorption by soil, water, stone, and plants. The lifetime of sulfur dioxide in the atmosphere is estimated to range between

20 minutes and 7 days (Nordo, 1973). Following is a discussion of the various mechanisms mentioned.

Vegetation: A portion of the much needed sulfur used by plants in metabolic processes has been shown by Fried (1948) to be attributed to the direct absorption of SO_2 from the atmosphere, especially in areas where the soil is sulfur deficient. The ability of the plant to utilize this sulfur effectively without damage is dependent upon the rate of absorption of SO_2 and the rate of production of sulfites.

Studies by de Cormis (1969) suggested that the extent of SO_2 absorption is directly proportional to the atmospheric SO_2 concentration and is not influenced by the amount of sunlight. Hill (1971) investigated the uptake rates of several gases by an alfalfa canopy. His results [see Figure 1] confirmed those of de Cormis. Hill found that SO_2 was absorbed with a deposition velocity of 2.8 cm/sec, given a wind velocity of 1.8-2.2 m/sec as well as a number of other fixed variables. He did note that, in general, those gases readily absorbed by the alfalfa were those with the greatest solubility in water [see Table II].

Table II. SOLUBILITY IN WATER AND UPTAKE RATE OF POLLUTANTS

Pollutant	Uptake Rate in Alfalfa* (mol/m ² sec) x 10 ⁹	Solubility at 20° C g/100 g
CO	0	0.00234
NO	2.1	0.00625
O ₃	34.7	0.052
NO ₂	39.6	decomposes
SO ₂	59.0	10.8

*Concentration of the gas in the chamber was 2×10^{-6} mol/m³.

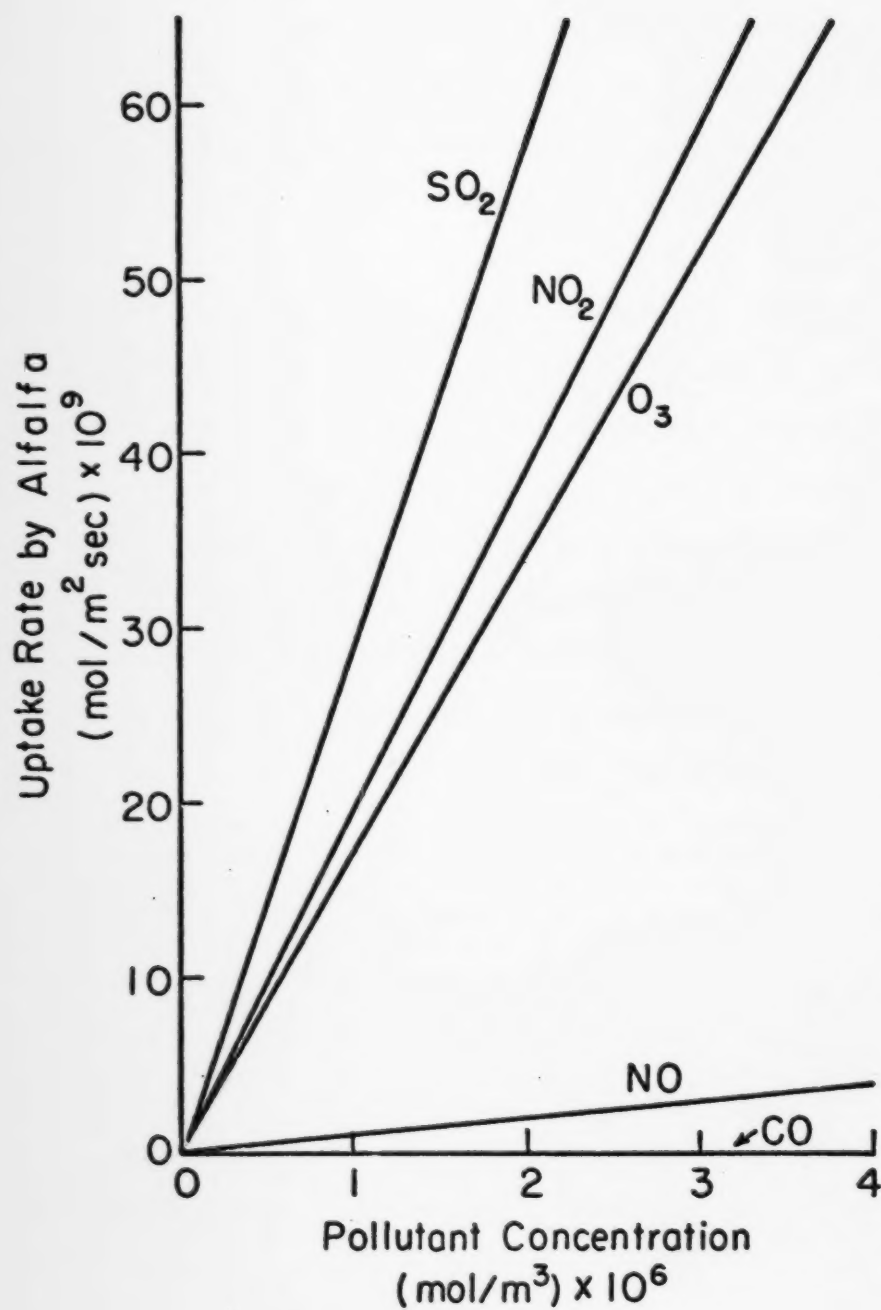


Figure 1. Uptake rates of different pollutants by an alfalfa canopy.

Factors which influence pollutant uptake by plant canopies have been discussed by Bennett and Hill (1973). In a more recent communication Bennett et al. (1973) present a model simulating pollutant transfer between leaves and the free air surrounding it. This model is based on the rate of exchange via a series of external and internal leaf mass transfer resistances. The model indicates the importance of gas solubility within the leaf.

Estimates of the amount of SO_2 removed each year by vegetal absorption vary greatly. Eriksson's (1963) cycle estimates 75×10^9 kg SO_2 -S are removed in this manner. Junge (1963) estimates 70×10^9 kg SO_2 -S, Robinson and Robbins (1968) estimate 26×10^9 kg SO_2 -S, Kellogg et al. (1972) estimate 15×10^9 kg SO_2 -S, and Friend (1973) also estimates that 15×10^9 kg SO_2 -S are absorbed by vegetation each year. The designation " SO_2 -S" expresses the mass of sulfur existing in the SO_2 form.

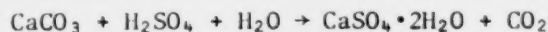
Soil: Various studies have shown that soils are capable of absorbing significant amounts of sulfur dioxide (Vandecaveye, 1936; Bohn, 1972). Terraglio and Manganelli (1966), in studies of two soil types, found not only that SO_2 was more readily absorbed by soil with a higher moisture content, but that the reaction also appeared to be dependent upon the pH of the soil, more SO_2 being absorbed in the soil where the pH was greater. The degree of absorption is also dependent upon such factors as the mineral and organic content of the soil, soil structure, ion-exchange capacity and porosity (Faller, 1968; Seim, 1970; and Smith et al., 1973). Both Seim and Smith et al. suggest that the SO_2 absorbed is oxidized to sulfate which may then be subject to leaching and/or plant uptake.

Deposition velocities have often been used to determine the removal

of SO_2 from the air above soils and vegetation. From the data available in the literature deposition velocities for soils are in the range of 0.2 - 0.7 cm/sec, which seem to be less than those for vegetation (Chamberlain, 1960; Spedding, 1969a; and Owers and Powell, 1974).

Estimates on the amount of SO_2 that is absorbed by soils are lacking and, for the most part, missing from most sulfur cycles that have been compiled. Unless this process has been taken into account in estimating the total sulfur deposited by dry deposition on the land surface then one must conclude that there is an obvious omission in the cycles. Eriksson (1963) estimated that 25×10^9 kg SO_2 -S per year are directly absorbed by the soil. Abeles et al. (1971), based on experiments they themselves ran, concluded that soils of the United States are capable of removing 4×10^9 kg of SO_2 per year (2×10^9 kg SO_2 -S).

Stone: Sulfur dioxide in the atmospheric environment has caused inestimable damage to frescoes, monuments and other edifices throughout the world. The damage is a result of enhanced weathering rates caused by the attack of sulfuric acid ($\text{SO}_2 + 1/2 \text{O}_2 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{SO}_4$) on the carbonate matrix of limestone and sandstone. Spedding (1969b) showed that the SO_2 uptake rate is dependent upon the moisture level in the atmosphere. The H_2SO_4 reacts with the carbonate matrix to form gypsum as follows:



(Luckat, 1973). Because the resulting salt is more soluble in water than the carbonate, the gypsum would be more readily leached out from the stone. The stone would also be subject to physical disintegration because of the volume expansion that accompanies the mineral change (Luckat, 1973).

Luckat also points out that the extent of weathering varies with the porosity of the affected rocks as well; a rough, porous, lime-cemented

sandstone would weather faster than a smooth and dense limestone.

Luckat (1973) and Spedding (1969b) provide values for SO_2 removal by stone of 6 - 200 and 50 - 200 $\text{mg/m}^2 \cdot \text{d}$, respectively. Luckat's data were obtained in highly industrial sections of Germany and Spedding had a concentration of $360 \mu\text{g SO}_2/\text{m}^3$ (100 times the world-wide background level) in his experiments. Taking $5 \text{ mg/m}^2 \cdot \text{d}$ as the lower limit of these data, the total earth's surface of $5 \times 10^{14} \text{ m}^2$, and an estimate that one percent of the earth's surface is stone capable of removing SO_2 , the annual removal rate is calculated to be $4.5 \times 10^9 \text{ kg S/yr}$. By comparison to Table IV this rate is considerably smaller than any of the estimated rates for the other natural SO_2 sinks.

Water Bodies: Theoretical discussions in support of the contention that sea water is capable of absorbing significant quantities of sulfur dioxide from the atmosphere first appeared in a paper by Liss (1971). He showed that the exchange of SO_2 across an air-liquid boundary is controlled by the resistance of the gas-phase and is a function of the pH of the aqueous solution.

Liss and Slater (1974) elucidated and modified the theory suggested by Liss (1971). Liss and Slater used the mass transfer coefficient for water vapor to calculate the overall mass transfer coefficients for a number of gases crossing the air-sea interface. The results are given in Table III. To calculate the SO_2 flux across the air-water interface, one must know the SO_2 solubility. An equation to predict this parameter at low SO_2 concentrations is now available (Hales and Sutter, 1973).

Estimates of the amount of SO_2 absorbed annually by the oceans indicate the importance of this sink. Liss and Slater (1974) estimate this

Table III. MASS TRANSFER COEFFICIENT FOR A NUMBER OF GASES
CROSSING THE AIR-SEA INTERFACE

Gas	k_g cm/sec	k_l cm/sec	H	r_g/r_l	K^* cm/sec
SO ₂	0.45	9.6	3.8×10^{-2}	573	0.45 (g)
N ₂ O	0.53	0.0055	1.6	6.6×10^{-3}	0.0055 (l)
CO	0.67	0.0055	50	1.7×10^{-4}	0.0055 (l)
CH ₄	0.885	0.0055	42	1.5×10^{-4}	0.0055 (l)
H ₂ O	0.833	∞	---	∞	0.83 (g)

*The overall exchange constant, K, is expressed on either a gas (g) or liquid (l) phase basis.

SO₂ flux at 1.5×10^{11} kg/yr based upon their own calculations. Their estimate is in good agreement with those of Eriksson (1963) (2×10^{11} kg/yr) and Robinson and Robbins (1968). (0.5×10^{11} kg/yr), but is lower than that determined by Spedding (1972) (9.6×10^{11} kg/yr). Liss and Slater explain that this discrepancy is due to a $3 \mu\text{g}/\text{m}^3$ difference in the mean atmospheric SO₂ concentration used by each and because Spedding's value for the total resistance of the gas phase ($1/K_g$) was much lower. As noted earlier, Kellogg *et al.* (1972) consider the net flux of SO₂ from air to sea to be negligible, based on observations made by Pate *et al.* (personal communication to Kellogg *et al.*) that in some areas, where the equilibrium vapor pressure of SO₂ in surface waters exceeds the partial pressure of SO₂ in the air above it, the ocean might actually be a source of SO₂.

Washout and Rainout of SO₂: The major portion of SO₂ present in the atmosphere is probably removed by the processes known as rainout and washout. Rainout involves the scavenging of SO₂ and sulfate particles within the clouds while washout is the removal of these sulfur compounds

below cloud level via precipitation. The SO_2 scavenged will undergo a series of reactions, some catalytic, and ultimately form H_2SO_4 drops or a sulfate salt. From the time SO_2 is absorbed by cloud droplets it is both ionized and oxidized by the reaction sequence suggested by Scott and Hobbs (1967).

Because the oxidation of SO_2 in the liquid phase does not occur at a rate fast enough to account for the sulfate content found in rain, investigations were undertaken to find an effective catalyzing agent. Experiments have shown that of all the metals found in the atmosphere, Mn salts were the most effective in promoting SO_2 oxidation (Junge and Ryan, 1958; Johnstone and Coughanowr, 1958; Matteson *et al.*, 1969). Although Mn salts are the best known catalyst for SO_2 oxidation, the concentration of these salts in the atmosphere is still not great enough to account for the sulfate content in rain. Recent investigations have shown that when ammonia is present the rate of sulfate production in solution is greatly enhanced (van den Heuval and Mason, 1963; Scott and Hobbs, 1967; Miller and de Pena, 1972)

Field investigations by Beilke and Georgii (1968) indicated that the absorption of gaseous SO_2 by rainout and washout accounted for 75% of the sulfate content in rain water and that scavenging of sulfate particles contributed only 25%. The model formulated by Miller and de Pena contradicts those measurements of Beilke and Georgii. Miller and de Pena show that the sulfate content of rainwater is much more dependent on the scavenging of particles rather than SO_2 . In their model, the sulfate content of rain water near a highly concentrated SO_2 plume of only moderate particle concentration showed that the contribution of SO_2 to the total sulfate concentration was 4 times less than that of sulfate particles.

Appreciable effort has been devoted to the analysis of SO_2 scavenging

by rain (Engelmann, 1968; and Fuquay, 1970). Field measurements of SO_2 washout (Hales et al., 1971) have demonstrated that there is a significant accumulation of SO_2 in the water drops.

A comprehensive analysis of reversible washout based on the interaction of raindrops with atmospheric contaminants has been presented by Hales (1972). This analysis indicates the use of overall mass transfer coefficients for determining the washout. From this analysis, it is apparent that the degree of success in determining washout rates depends on estimating mass transfer coefficients and solubility data. Further study (Hales et al., 1973a and Hales et al., 1973b) has led to the development of a mathematical model for predicting ground level concentrations in the rain as a function of location beneath a plume under stable meteorological conditions.

Atmospheric Reactions Involving SO_2 : Reactions involving SO_2 in the dry state, not unlike those discussed above for SO_2 in the wet state, are very complex. The most important reaction involved here is the photochemical oxidation of SO_2 which takes place in polluted atmospheres.

Early measurements of the rate of photo-oxidation of SO_2 made by Gerhard and Johnstone (1955) seem to be the most widely quoted. They found the rate of SO_2 oxidation to proceed from 0.1-0.2%/hour. Renzetti and Doyle (1960) and Cox and Penkett (1970) have suggested that the rate of photochemical aerosol formation (the end result of the photo-oxidation of SO_2) is greatly accelerated in the presence of olefinic hydrocarbons and nitric oxide. Endow et al., (1963) and Harkins and Nicksic (1965) have shown that the resulting aerosols consist almost entirely of sulfuric acid droplets when the relative humidity is greater than or equal to 50%.

Cox and Penkett (1971a) have given experimental evidence to support the hypothesis that low concentration olefinic hydrocarbons and nitric

oxide can greatly affect the rate of SO_2 photo-oxidation in air. Results of their experiments can be easily observed from Figure 2.

Although the rate of SO_2 oxidation by ozone alone is quite slow, Cox and Penkett (1971b) found that when SO_2 was injected into a chamber containing ozone and olefins the oxidation rate was greatly enhanced. They also found that the oxidation rate, or aerosol formation, was dependent upon the nature of the olefin.

As little as is known about the oxidation of SO_2 in the troposphere, still less is known about its oxidation in the stratosphere. Kellogg et al. (1972) have suggested a possible 3-body reaction with atomic oxygen for removal within the stratosphere:



where M is a molecule of O_2 or N_2 , which acts to carry off the excess energy, thereby preventing prompt reversal of this reaction. The SO_3 formed reacts almost immediately with H_2O vapor to form H_2SO_4 which then combines with more water to form droplets of H_2SO_4 solution which are then removed by precipitation. This reaction is thought, by the authors, to be responsible for the layer of H_2SO_4 or sulfate particles found at an altitude of approximately 18 km.

Perhaps the best way to summarize the possible reactions involving SO_2 in the atmosphere would be by repeating the summary made by Robinson and Robbins (1968). "It seems that in the daytime and at low humidity, photochemical reaction systems involving SO_2 , NO_2 and hydrocarbons are of primary importance in the transformation of SO_2 into essentially an H_2SO_4 aerosol. At night and under high humidity or fog conditions, or during actual rain, it seems that a process involving the absorption of $\text{SO}_4^{=}$ by alkaline water droplets and a reaction to form $\text{SO}_4^{=}$ within the

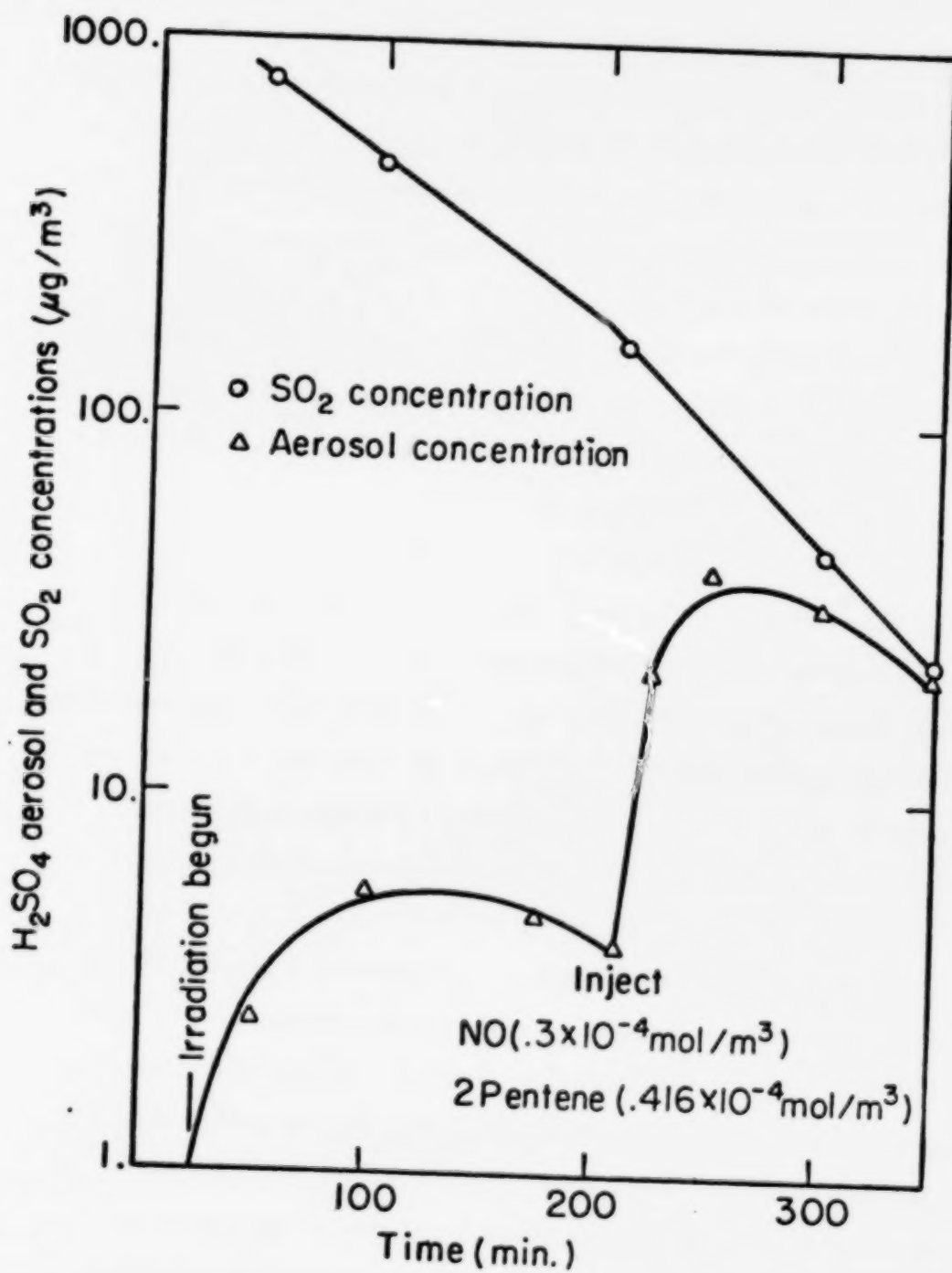


Figure 2. Aerosol formation and SO_2 decay during the photooxidation of SO_2 .

drop... can occur at an appreciable rate to remove SO_2 from the atmosphere."

Environmental Sulfur Cycle

Table IV summarizes the estimates made by Eriksson (1960), Junge (1963), Robinson and Robbins (1968), Kellogg et al. (1972) and Friend (1973) in compiling their respective sulfur cycles. It should be kept in mind that while all the values given are only estimates, the degree of uncertainty in some is greater than that in others. For instance, there are no measurements upon which estimates of the quantity of H_2S or $\text{S}^\pm$ emitted by decaying land and sea biota can be based. Also, there are no specifications of the form of the sulfides (i.e. H_2S , HS^- , or $\text{S}^\pm$). These estimates have therefore been arrived at by the authors' balancing of particular portions of their cycles; the difference needed to balance each section has then been set equal to the flux of H_2S or $\text{S}^\pm$ from the land and sea to the atmosphere, respectively.

CARBON CONTAINING GASES

CARBON MONOXIDE

Each year more carbon monoxide is released into the atmosphere than any other pollutant (excluding carbon dioxide), and, each year the quantity released increases. One would therefore expect a gradual increase in ambient CO levels, yet one finds that the background concentration of this gas in the atmosphere has not fluctuated the last few decades. There must then be one or several major active sinks for CO within the troposphere. Until just a few years ago though, investigations on possible sinks had only turned up additional sources of CO. This dilemma, as a result, came to be known as the "CO sink anomaly".

Background concentrations of CO range from 50-200 $\mu\text{g}/\text{m}^3$ (0.04-0.20 ppm) (Jaffe, 1973). Robinson and Robbins (1968) indicate that a mean concentration of 100 $\mu\text{g}/\text{m}^3$ (0.1 ppm) is found in the northern hemisphere, while concentrations less than 60 $\mu\text{g}/\text{m}^3$ (0.05 ppm) would probably be more common in the southern hemisphere.

Sources

Carbon monoxide is the product of incomplete combustion of fossil fuels containing carbon. With the advent of large scale industrialization and the tremendous increase in the use of the automobile, great quantities of CO have been emitted into the atmosphere. Recent investigations for CO sinks to explain why the ambient CO concentration has not been increasing have resulted in the discovery of new natural sources of CO whose total quantity far exceeds the total mass of CO produced as a result of man's technology (Stevens et al., 1972).

By far the greatest single anthropogenic source of CO is motor

vehicle exhaust. Jaffe (1973) estimated a total anthropogenic CO emission source in the United States in 1970 of 132.6×10^9 kg and 359×10^9 kg on a global scale. He notes that whereas the level of CO produced by man in the United States appears to be leveling off, globally it is on an increase. Underdeveloped nations, which are undergoing increased technological development, are not as yet concerned with the resulting pollution as much as the economic gains and so their emission levels are on the rise.

The most widely recognized natural source of CO is forest fires which have been estimated as releasing 11×10^9 kg CO into the atmosphere each year (Robinson and Robbins, 1968). This is, by no means, the only major natural source of CO. Minor amounts of CO have been found to be released from volcanoes and marshes (Flury and Zernik, 1931). CO can also be formed during electrical storms (White, 1932) and by the photodissociation of CO_2 in the upper atmosphere (Bates and Witherspoon, 1952). Calvert et al. (1972) has suggested the photodissociation of formaldehyde as a possible source of CO and recently, Swinnerton et al. (1971) have found CO to be present in rain water in rather high concentrations. Galbally (1972) has offered a hypothesis wherein the CO in rain is a product of the photodecomposition of aldehydes in the rain water by sunlight.

The ocean was first suggested as a major source of CO by Swinnerton et al., (1970). Linnenbom et al., (1973) have estimated the oceans can produce up to 220×10^9 kg each year, whereas Liss and Slater (1974) have estimated this flux at 43×10^9 kg per year. Robinson and Moser (1971) have suggested that plants could indirectly be the source of about 54×10^9 kg CO by the oxidation of released terpenes. Finally, McConnell et al., (1971) suggested that approximately 900×10^9 kg CO are produced

each year by the oxidation of methane.

In light of this new source information, Stevens et al. (1972) believe that natural sources of carbon monoxide could yield about 10 times more CO than all anthropogenic sources in the northern hemisphere. Up to this time it has been assumed that anthropogenic activity released far more carbon monoxide than nature. It will be interesting to follow the outcome of this contradiction over the next few years.

Removal Mechanisms

Carbon monoxide can be regarded, for all intents and purposes, as being insoluble in water; its actual solubility being only 0.00234g CO/100g H₂O at 20°C. Therefore, wet processes such as washout and rain-out can be regarded as playing an insignificant part in the removal of CO from the atmosphere. Experiments on the absorption rate of CO by an alfalfa canopy (Hill, 1971) showed that virtually no CO was absorbed and therefore, vegetation can be disregarded as a sink. Absorption of CO by the oceans can now be disregarded as well because it has recently been shown (Swinerton et al., 1970) that the oceans actually constitute a significant natural source of carbon monoxide. It seems then that the major sinks for CO are gas-phase reactions in the troposphere and stratosphere and soil fungi (Inman et al., 1971; and Inman and Ingersoll, 1971). Estimates of the residence time of CO in the troposphere range from about 0.1 year (Weinstock, 1969) to about 2.7 years (Robinson and Robbins, 1968).

Soil: Experiments by Inman and Ingersoll (1971) showed that both potting soils and natural soils absorbed from 2-20 mg CO/m²·hr. They observed that, in general, soils with the highest uptake activity were those with higher organic content and lower pH. Inman et al. (1971) also noted that if a soil was autoclaved (sterilized) removal of CO by the soil was

inhibited. This suggested that the removal was due to biological activity in the soil.

In late 1972 Ingersoll published the results of a more extensive study on the uptake of CO by soils. Here he measured the in situ uptake at various locations throughout North America. He found that:

1) The total amount of CO destroyed by various soils ranged from 7.5 to 109.0 mg CO/hr·m², the spectrum ranging from tropical soils which were the most active down to desert soils which were the least active. Although there were many exceptions, more CO tended to be destroyed by soils with low pH and moderate moisture content (~20%) than others.

2) The rate of CO uptake decreased as the concentration of CO decreased in the air, with maximum removal with ambient concentrations of 100,000 µg/m³ (100 ppm).

3) Given the same soil, CO uptake was far greater when vegetation was growing than when the soil was under cultivation. Ingersoll suggests this is because the amount of organic matter present in soils being cultivated is substantially lower than that present in soils actively growing crops.

4) Soils that were removed from their site of origin and tested in the laboratory showed greatly reduced uptake ability. The magnitude of decrease was not uniform from one soil sample to the next.

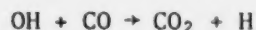
Based upon data he had collected which he corrected for temperature and uptake variations, Ingersoll (1972) estimated the CO uptake potential of the conterminous United States and the world. His estimates of 505×10^9 kg and 14.3×10^{12} kg CO per year for each, respectively, are based on ambient CO levels of 100,000 µg/m³ (100 ppm), three orders of magnitude

greater than average ambient CO levels. Ingersoll noted that Seiler (1972) had found soil CO uptake rates to be one-tenth of those Ingersoll had measured when these soils were exposed to ambient CO levels (200-1000 $\mu\text{g}/\text{m}^3$) rather than concentrations of 100,000 $\mu\text{g}/\text{m}^3$. On the basis of this information, Ingersoll reduced his estimates of the total capacity of soils to consume CO in the United States and the world to around 50×10^9 kg and 1.4×10^{12} kg per year, respectively.

Earlier, Inman and Ingersoll (1971) had estimated that soils of the continental United States were capable of removing over 500×10^9 kg CO per year.

Results of recent experiments by Smith et al. (1973) support earlier findings that soils are capable of effectively removing CO from the atmosphere. They also found though that when moist soils were placed in the chamber with air containing 100,000 $\mu\text{g CO}/\text{m}^3$ (100 ppm), the concentration of CO in the chamber rose, in one case tripled, before it was reduced to zero. This effect was found to be more pronounced in sterilized soils than unsterilized soils. They surmise that the evolution of CO from the soils is a nonbiological process, but made no attempts to identify the processes responsible.

Atmospheric Reactions Involving CO: Recently it has become apparent that the stratosphere constitutes a sink for carbon monoxide. The significant reaction seems to be the reaction of CO with the hydroxyl radical (Weinstock, 1969; Pressman and Warneck, 1970; and Pressman et al., 1970) as follows:



A rate constant for this reaction is available (Schofield, 1967). The series of reactions which follow not only provide for the regeneration

of the OH radical needed but possibly for the reaction of CO with the hydroperoxyl radical as well (Westenberg and de Haas, 1972; and Davis et al., 1973).

Vertical CO profiles of the atmosphere have recently been carried out by Seiler and Junge (1969), and Seiler and Warneck (1972). These reports both found a sharp decrease in the CO mixing ratio when crossing the tropopause into the stratosphere. The mixing ratio is defined as the mass of gas per unit mass of dry air. It seems obvious from vertical profiles such as these that there is a significant decrease in the CO concentration above the tropopause, thus rendering valid the conclusion that the stratosphere is a sink for carbon monoxide.

Quantitative estimates of the amount of CO destroyed in the stratosphere by this reaction mechanism have not been made. Pressman and Warneck (1970) believe that virtually all CO entering the stratosphere is destroyed in that manner. Therefore, the size of the stratospheric sink is dependent upon the transport rate of CO rich air through the tropopause into the stratosphere. They have estimated this flux at 1.3×10^{-3} mol/m²·sec but admit the degree of uncertainty in this estimate is very high due to insufficient data. Based on this flux and recent estimates of the total CO reservoir in the troposphere, they estimated that about 11-15% of the total CO inventory in the troposphere is destroyed in the stratosphere.

Although the reaction sequence mentioned above has been recognized as a major sink in the stratosphere, only recently has it been suggested to be a significant destructive reaction in the troposphere (Weinstock, 1969). Recent investigations (Levy, 1971; and McConnell et al., 1971) have shown that great enough concentrations of hydroxyl and hydroperoxyl

radicals also exist in the troposphere to provide a mechanism for the oxidation of carbon monoxide there too.

Carbon Monoxide Cycle

Over the last several years we have witnessed an explosion of interest in the problem of defining natural sources and sinks of carbon monoxide. While several researchers have confirmed that soil and the reaction of CO with hydroxyl and hydroperoxyl radicals in the stratosphere and possibly the troposphere constitute major sinks for CO, other researchers have been finding additional natural sources of this gas. These sources, oxidation of methane, oxidation of terpenes, and the oceans to name just a few, are now thought to contribute more CO to the atmosphere than that emitted as a result of anthropogenic activity. This is an outright contradiction of what only two years ago was thought to be the final word; i.e., anthropogenic CO emissions are many times greater than natural CO emissions.

Table V compares recent estimates of the strength of CO sources and sinks. It is obvious from this table, if these estimates are at all reasonable, that soil and gas-phase oxidation in the stratosphere and troposphere might be capable of consuming all the CO that nature and man produce. If this is the case, it is understandable why the background concentration of CO has not increased over the last several decades, and we might suggest that there no longer exists a "CO sink anomaly".

Table V. ATMOSPHERIC FLUXES OF CARBON MONOXIDE (in 10^9 kg/yr)

I. Sources

a.	anthropogenic	359	Jaffe (1973)
b.	natural		
1.	oceans	43-220	Liss and Slater (1974) - Linnenbom <u>et al.</u> (1973)
2.	oxidation of terpenes	54	Robinson and Moser (1971)
3.	oxidation of methane	900	McConnell <u>et al.</u> (1971)
4.	other	<u>?</u>	
	TOTAL	1356-1533	

II. Sinks

a.	soil	67-1400	Heichel (1973) - Ingersoll (1972)
b.	gas-phase oxidation		
1.	stratosphere	52-71	Pressman and Warneck (1970)
2.	troposphere	<u>?</u>	
	TOTAL	119-1471	

NITROGEN CONTAINING GASES

Although the most abundant oxide of nitrogen in the lower atmosphere is nitrous oxide (N_2O), it does not play an important part in air pollution chemistry. The two nitrogen oxides which are important are nitric oxide (NO) and nitrogen dioxide (NO_2) for they play a prominent role in the generation of photochemical smog.

Measurements of the background levels of nitrous oxide seem to consistently average out to about $460 - 490 \mu\text{g}/\text{m}^3$ ($0.25 - 0.27 \text{ ppm}$) (Schütz *et al.*, 1970). Ambient levels of NO_2 are much lower, probably around $2 \mu\text{g}/\text{m}^3$ ($.001 \text{ ppm}$) (Robinson and Robbins, 1968) to $2.6 \mu\text{g}/\text{m}^3$ ($.0014 \text{ ppm}$) (Junge, 1963). Too few accurate measurements have been made of ambient concentrations to obtain a meaningful average but Lodge and Pate (1966) found concentrations up to $11 \mu\text{g}/\text{m}^3$ ($.006 \text{ ppm}$) in Panama. The background level of NO is approximately the same as that of NO_2 .

The other nitrogen compound considered is ammonia. Although ammonia, *per se*, is a relatively unimportant air pollutant, it does play an important role in atmospheric chemistry for its part in the formation of aerosols. Ambient concentrations of ammonia seem to average about $4 \mu\text{g}/\text{m}^3$ ($.006 \text{ ppm}$) (Robinson and Robbins, 1968).

NITROGEN OXIDES

Sources

Nitrous oxide (N_2O), which is the most abundant nitrogen compound present in the atmosphere, is produced as a result of the decomposition of other nitrogen compounds within the soil by bacteria. Arnold (1954) was the first to study the production of N_2O by soils. He found that the one factor most conducive to increased N_2O evolution is a high soil moisture content, especially if a nitrogen source, such as nitrate or ammonia, is present. An estimate of the flux of N_2O from soils into the atmosphere

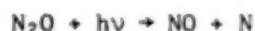
has recently been made by McConnell (1973), who estimates that 1.1×10^{10} kg $\text{N}_2\text{O} - \text{N}$ (1.73×10^{10} kg N_2O) are released each year; Schütz *et al.* (1970) declined to extrapolate the data they collected on three soil samples to attain a global rate. Their measurements though showed a flux on the order of 10^{-8} g $\text{N}_2\text{O}/\text{m}^2 \cdot \text{sec}$, an order of magnitude which, if maintained globally, would necessitate an N_2O residence time of about 70 years. This is the same residence time they had estimated based on the photodissociation rates of N_2O in the troposphere and stratosphere. Goody and Walshaw (1953) estimated the N_2O global production rate to be about 100×10^{12} kg/yr and Robinson and Robbins (1970) estimated that soils produce about 59.2×10^{10} kg N_2O each year by this biological action; of this about 55.4×10^{10} kg (35.3×10^{10} kg $\text{N}_2\text{O}-\text{N}$) are reabsorbed by the soil and about 3.8×10^{10} kg N_2O (2.4×10^{10} kg $\text{N}_2\text{O}-\text{N}$) travels up to the stratosphere where it is destroyed. It is the latter rate that is shown in Table VI.

Craig and Gordon (1963) raised the possibility that the ocean might be a source or a sink of N_2O . Bates and Hays (1967) concluded that the uptake of N_2O by the oceans in areas where upwelling waters are deficient in N_2O is of negligible importance. Based upon the difference between the mean N_2O concentrations of oceanic surface waters and the air about it and an estimate of the total liquid phase resistance, Liss and Slater (1974) estimated the flux of N_2O from the ocean to the atmosphere at 1.2×10^{11} kg/year. This flux is based entirely on theory and not measurements, but it does indicate that the oceans could conceivably release significant quantities of N_2O to the atmosphere. Laboratory and field experiments should be undertaken to provide an answer as to whether or not the ocean is a source of N_2O .

Production rates of NO and NO_2 by soils are much more difficult to measure and estimate, and good data are lacking. McConnell (1973) recently summarized a few of the problems involved in obtaining an estimate for the amount of nitrogen oxides produced by soil. It is his contention that

this soil source is small compared to the production resulting from the gas phase oxidation of atmospheric ammonia by OH which he estimates produces 7×10^{10} kg $\text{NO}_x - \text{N}$ per year. McConnell though offers alternative reaction sequences for NH_3 in the atmosphere; one reaction sequence provides a constant source of NO, the other a sink. If the latter is shown to occur in the atmosphere, then an additional or enlarged source of NO must be found in order to account for the amount of NO known to be in the atmosphere. If this is the case, McConnell concedes that the soil might actually constitute a significant source of NO_x , on the order of 10^{11} kg/yr.

Nitric oxide is also produced as a result of the photolysis of N_2O in the stratosphere as follows:



The photolysis rate for this reaction is less than or equal to 7.4×10^{-9} sec^{-1} (McElroy and McConnell, 1971). Whereas these authors estimate the production of about 3×10^8 kg $\text{NO}_x - \text{N}$ per year in this manner, Bates and Hays (1967) estimated that 3.5×10^{10} kg NO are produced annually by this photolysis reaction.

The other primary source of nitrogen oxides is anthropogenic, primarily combustion processes. Estimates of production rates for NO and NO_2 are included together because emission data available rarely distinguish between these two forms. Robinson and Robbins (1970) recently estimated that each year 18×10^9 kg $\text{NO}_x - \text{N}$ are emitted into the atmosphere as a result of man's activities. An earlier estimate by these same men in 1968 states that 53×10^9 kg of NO_2 were emitted annually (here again NO_2 includes both NO and NO_2 production).

In toto, natural emissions of NO_2 (including NO) are approximately 15 times greater than anthropogenic emissions (768×10^9 kg vs. 53×10^9 kg

NO₂) (Robinson and Robbins, 1970). Therefore anthropogenic emissions play only a minor part in the total circulation of nitrogen compounds in the atmosphere.

Removal Mechanisms

At 20°C, the solubility of N₂O in water is 0.121 g/100g H₂O. Upon release from soils, an unknown portion is believed to be removed by vegetation, soil and water. No information is available on these processes though. The major portion of the released N₂O is destroyed by photodissociation in the stratosphere and upper troposphere. Because under normal tropospheric conditions N₂O is chemically inert, it partakes in no other chemical reactions in the troposphere. The residence time of nitrous oxide is probably around 70 years if there is no removal by the biosphere (Robinson and Robbins, 1968), but could be reduced to about 1-3 years if there is a biologic loss mechanism. Hidy (1973) has estimated the residence time as 4 years.

Nitric oxide is rather insoluble in water. At 20°C its solubility is 0.00618 g/100g H₂O. Nitrogen dioxide, on the other hand, immediately dissociates when in water to form HNO₃ and HNO₂. For this reason, no real value for the solubility of NO₂ in water exists.

Nitric oxide is either oxidized to NO₂ or photolyzed to N₂. The NO₂ is then removed primarily by precipitation, more often than not in the form of nitric acid (HNO₃). NO₂ can also be absorbed by vegetation and soils or participate in photochemical reactions to form aerosols. Due to their reactivity, the residence times of NO and NO₂ are relatively short, probably around 5 days (Hidy, 1973). Nitrogen oxides are removed from the atmosphere by the following mechanisms.

Vegetation: Vegetation has been shown capable of removing significant

amounts of NO_2 and NO from the atmosphere. Tingey (1968) showed that alfalfa and oats absorbed NO_2 from the air in excess of $100 \times 10^{-12} \text{ mol/m}^2 \cdot \text{sec}$ when exposed to an atmosphere containing $460 \text{ } \mu\text{g NO}_2/\text{m}^3$ (or $\sim 1 \times 10^{-5} \text{ mol/m}^3$).

Hill (1971) found in his experiments on the uptake rate of gases by an alfalfa canopy that NO was absorbed with a deposition velocity of 0.1 cm/sec , and NO_2 with a velocity of 2 cm/sec when present in the air of the chamber at a concentration of $2 \times 10^{-6} \text{ mol/m}^3$ (or $96 \text{ } \mu\text{g/m}^3$).

Soil: Nitrogen oxides (especially N_2O) have long been known to be produced by biological action in soils. Recently though, Abeles et al. (1971) found that soils could absorb nitrogen dioxide from the atmosphere as well. Extrapolating the results of their experiment, the authors suggest that the soils of the United States might be capable of removing $60 \times 10^{10} \text{ kg}$ of NO_2 per year from the atmosphere, an amount they point out to be a bit under 20 times the total annual production of NO_2 in this country ($3.3 \times 10^{10} \text{ kg}$).

Nelson and Bremner (1970) point out that the NO_2 that the soil absorbs will ultimately be oxidized to nitrate. These nitrates eventually decompose and result in the production of nitrogen dioxide again. The rate of NO_2 production by nitrate decomposition in soils is $2 \times 10^{-4} \text{ g NO}_2/\text{m}^2 \cdot \text{hr}$ (Marchesani et al., 1970; and Makarov, 1970, as cited in Bohn, 1972). This NO_2 production rate is dependent upon the nitrate content of the soil and does not proceed during darkness.

Nitric oxide may also be absorbed by soils, but upon absorption is oxidized almost immediately to NO_2 (Mortland, 1965; and Bremner and Nelson, 1968). Mortland has also discovered that when transition metal ions

are present in the soil, absorption of NO is promoted. If the soil is saturated with alkaline earth cations though, absorption of NO is halted. Sundareson *et al.* (1967) found though that alkaline-earth zeolites readily absorb NO and released it as NO_x and HNO₃ when heated. To date, the role organic matter plays in the absorption of nitrogen oxides by soil remains a mystery. Ganz *et al.*, (1968, as cited in Bohn) found that upon passing NO_x-contaminated air through 1 meter of peat, all nitrogen components were removed. Organic matter is such an important component of soil that to not be fully aware of its affects on a gas could only hinder full understanding of the mechanism of absorption by the soil. Obviously, more research is needed in this area.

Water Bodies: There are very little data available on the amount of nitrogen oxides absorbed by the oceans. Craig and Gordon (1963) first suggested that the oceans might constitute a sink for N₂O when they found that the sea water at depth was depleted in N₂O compared to the surface waters which they found to be in equilibrium with atmospheric concentrations. The depletion they determined could not be explained by temperature variations with depth. Based on the mean upwelling speed of the ocean's waters, estimated by Bowden (1965) as ranging from 10⁻⁴ to 10⁻⁵ cm/sec, Bates and Hays (1967) estimated the potential sink strength of the oceans for N₂O as ranging between 6 x 10⁻⁷ and 6 x 10⁻⁶ kg/m².yr. Liss and Slater (1974), on the other hand, concluded that the flux of N₂O was from the sea to the air. They calculated a flux rate of 3.2 x 10⁶ kg/m².yr based upon an N₂O concentration gradient across the air-sea interface measured by Junge and Hahn (1971). The total flux of N₂O from the sea to the atmosphere, assuming this flux is constant over the entire oceanic surface, is 1.2 x 10¹¹ kg/yr. With such an obvious

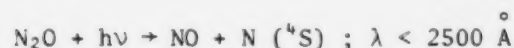
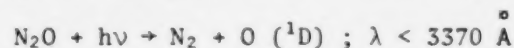
contradiction as to the direction of the N_2O flux, there is a real need for additional research in this area.

Washout and Rainout: The major sink identified thus far for nitrogen oxides (NO_x) is the solution of soluble species in cloud and rain droplets with subsequent removal by precipitation. Different schemes of NO_2 hydrolysis have been proposed by Haagen-Smit and Wayne (1968), Georgii (1963) and Robinson and Robbins (1968). However the hydrolysis reaction proceeds though, the outcome is the same in all cases; the nitric acid formed is absorbed onto hygroscopic particles or reacts with atmospheric ammonia to form nitrate salt aerosols (NH_4NO_3 for instance). It is then either removed by precipitation, or if vaporization of the droplet occurs, by dry deposition.

McConnell (1973) estimates that 2×10^{10} kg $NO_3 - N$ is removed from the atmosphere each year by precipitation, and an additional 7×10^{10} kg $NO_x - N$ is removed by dry deposition, the major portion of this probably being HNO_3 .

Atmospheric Reactions Involving Nitrogen Oxides: Although more nitrous oxide is released to the atmosphere than any other nitrogen oxide it does not play a major or very complex role in atmospheric reactions. Because it is chemically inert in the troposphere, its sink lies in the stratosphere where it is transported by vertical mixing. In the stratosphere it is destroyed by photolyzing reactions.

Bates and Hays (1967) indicate that the most significant reactions are:

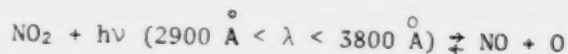


The latter reaction they believe to be responsible for about 20% of the total dissociation in the stratosphere.

Nitric oxide can be removed from the atmosphere by several reactions. The primary reaction is its oxidation by ozone to form NO_2 . In the upper atmosphere, NO can be photolyzed and the resulting atomic N may react with other NO molecules to form N_2 (Schofield, 1967; and Callear and Pilling, 1970).

Nitrogen dioxide also engages in a number of reactions. It may be oxidized to NO_3 (Schofield, 1967), or it may form nitric acid by its reaction with hydroxyl radicals (McConnell and McElroy, 1973). The nitric acid that is formed would be removed by precipitation. For further elaboration, the reader is referred to McConnell and McElroy's article.

The importance of NO and NO_2 as pollutants is a result of their participation in photochemical reactions. In polluted atmospheres they react with SO_2 and hydrocarbons to form aerosols. Probably the most important photochemical reaction involving NO_2 is its photodissociation as follows:



This atomic oxygen then is free to react with molecular oxygen to form ozone.

Peroxyl radicals ($\text{ROO}^{\bullet}$), formed by the reaction of reactive free radicals ($\dot{\text{R}}$) with O_2 , can react with NO and NO_2 to form alkyl nitrates or peroxyacyl nitrates. These secondary reaction products are then targets of further photochemical attack (Haagen-Smit and Wayne, 1968). Because it would not serve the purpose of this paper to elaborate on photochemical reactions involving nitrogen oxides, the reader is referred to Altshuller and Bufalini (1971), Cadle and Allen (1970), and Leighton (1961) for more detail.

Environmental NO_x Cycle

The circulation of nitrogen oxides in the atmosphere is a complex problem and, as yet, not well understood. The global NO_x cycles that have been formulated, those of Robinson and Robbins (1968) and McConnell (1973), have made it clear how very little good quantitative data exist. The holes in these cycles are obvious and major ones (see Table VI). We need, for instance, a better idea of how much NO and NO₂ is released from the soil, how much NH₃ is oxidized to NO_x, and how much NO and NO₂ is destroyed by photochemical reactions. And, we need to know why such a discrepancy exists between estimates that have been made and in ways they are made. For example, McConnell bases his estimate of NO_x removed by dry deposition on soil data, the nitrogen content of precipitation and a deposition velocity factor. Robinson and Robbins, on the other hand, use the deposition velocity function to estimate gaseous deposition, a removal mechanism McConnell makes no mention of. Inconsistencies like these indicate again the need for further study in this area.

AMMONIA

Sources

The primary source of atmospheric ammonia appears to be the result of bacterial decomposition of organic material on the earth's surface. The factors which affect the emission of this NH₃ from the soil are its nitrogen content, pH, and moisture content (McConnell, 1973; and Georgii, 1963). NH₃ is more readily released from dry soils than moist ones, and is more readily released when the pH of the soil is greater than or equal to 6. Junge (1963) also suggested that the oceans may contribute some NH₃ to the atmosphere, but to date there has been no accurate measurement made upon which to base an estimate of the source strength. McConnell

Table VI. ATMOSPHERIC FLUXES INVOLVED IN VARIOUS NO_x CYCLES (in 10¹⁰ kg N/yr)

	Robinson and Robbins* (1968)	Robinson and Robbins (1970)	McConnell (1973)
I. Sources			
a. anthropogenic; NO, NO ₂	1.5	1.6	1.8
b. biological; N ₂ O	1.2	1.2	1.1
c. biological; NO, NO ₂	30.4	23.4	?
d. oxidation of NH ₃	N.E.	N.E.	7
e. stratospheric transport; NO, NO ₂	---	---	0.07
TOTAL	33.1	26.2	9.97
II. Sinks			
a. rainout	112.9	7.5	2
b. dry deposition	27.1	1.9	7
c. oxidation of N ₂ O → NO (strat.)	0.2	0.2	0.03
d. photolysis of N ₂ O → N ₂ (strat.)	---	---	(1.07)
e. gaseous deposition	10.7	4.5	---
TOTAL	150.9	14.1	(10.1)

N.E. = Mechanism recognized but no estimate made.

*NOTE: Friend (1973) has pointed out that due to an error in converting units of kilograms per hectare to tons per square meter, much of Robinson and Robbins' nitrogen compound cycle is invalid. Friend though, gives no indication as to which values are wrong. Due to lack of information, their cycle is nonetheless shown for comparison.

has estimated that these biological sources release about 17×10^{10} kg NH_3 - N each year, whereas Robinson and Robbins' (1968) nitrogen cycle calls for the release of NH_3 on the order of 10^{12} kg NH_3 each year (see Table VII).

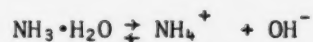
Anthropogenic NH_3 emissions result primarily from the combustion of coal. Robinson and Robbins (1970) estimated that the atmospheric ammonia burden due to man's activities is 0.4×10^{10} kg NH_3 - N per year, less than 2 1/2% of the estimated NH_3 burden due to biological emissions (17×10^{10} kg).

Removal Mechanisms

Ammonia is extremely soluble in water. At 20°C its solubility in water is 62.9 g/100g H_2O . From the data available, the residence time of ammonia in the atmosphere is probably around 7 days (Hidy, 1973).

Water Bodies, Vegetation, Soils, Atmospheric Reactions: Due to ammonia's solubility in water it can be readily absorbed by water bodies (Hutchinson and Viets, 1969; and Calder, 1972) and vegetation (Hutchinson et al., 1972; and Porter et al., 1972). Ammonia has also been shown to be readily absorbed by soils, especially acid soils (Malo and Purvis, 1964; DuPlessis and Kroontje, 1964; and Hanawalt, 1969a & b). It is also destroyed by its reaction with hydroxyl radicals in the atmosphere to form nitric oxide (McConnell, 1973).

Rainout and Washout: Probably the most important removal mechanism for ammonia is its solution in rain water along with SO_2 or other gases to form aerosols. Once dissolved NH_3 ionizes to NH_4^+ as follows (Robinson and Stokes, 1959):



Ammonia has been shown to be an important catalyst for the oxidation of SO_2 and NO_2 in solution (van den Heuval and Mason, 1963). Both Scott and Hobbs (1967) and Miller and de Pena (1972) have shown that as the partial pressure of NH_3 in the atmosphere increases, greater concentrations of SO_2 can be dissolved and oxidized in solution to form sulfate particles. The resulting aerosols, if evaporated, are composed largely of $(\text{NH}_4)_2\text{SO}_4$ particles with probably minor amounts of NH_4HSO_3 , NH_4HSO_4 and $(\text{NH}_4)_2\text{SO}_3$ (Miller and de Pena, 1972). In the case where NH_3 is co-absorbed with NO_2 , the resulting particles would be composed primarily of NH_4NO_3 .

It has been estimated (Robinson and Robbins, 1968) that almost 75% of atmospheric ammonia is removed from the atmosphere by conversion to NH_4^+ ions which condense in cloud droplets or particles and may form aerosols upon evaporation of water. McConnell (1973) has estimated that of a total NH_3 source strength of about 17.4×10^{10} kg NH_3 - N/yr, approximately 3×10^{10} kg of this ammonia are removed each year by rainout. He points out that this is a very conservative estimate and "may be low by as much as a factor of 3." Earlier, Robinson and Robbins estimated that 280×10^{10} kg NH_3 -N are removed each year by precipitation. On the whole, quantitative estimates are rather sparse and show a great discrepancy.

Environmental Ammonia Cycle

Relatively little quantitative information is available on the strengths of both sources and sinks of ammonia. In fact, research into possible atmospheric oxidation reactions is so recent that any estimates made would certainly be subject to great uncertainty. Separate atmospheric ammonia cycles have never been constructed; its cycle is always considered together with that of nitrogen oxides. Because not very much is even known about the nitrogen oxides cycles, the uncertainty involved in the combined cycle is probably very high.

To date the only nitrogen compound cycles devised are those of Robinson and Robbins (1968, 1970), McConnell (1973) and an overall geochemical nitrogen cycle of Rasmussen *et al.* (1974). The first three cycles are compared in Table VII. The discrepancy in source and sink estimates among the three is immediately obvious. More research must be undertaken to provide us with a better understanding of the part ammonia plays in atmospheric chemistry and to quantify possible sources and sinks such as the oceans, soil, and vegetation.

Table VII. ATMOSPHERIC FLUXES INVOLVED IN VARIOUS AMMONIA CYCLES
(in 10^{10} kg N/yr)

	Robinson and Robbins* (1968)	Robinson and Robbins (1970)	McConnell (1973)
I. Sources			
a. anthropogenic	---	.35	0.4
b. biological	<u>670±</u>	<u>95.7</u>	<u>17</u>
TOTAL	670	96.05	17.4
II. Sinks			
a. precipitation	280	18.6	3
b. dry deposition	70	4.9	7
c. oxidation to NO _x (troposphere)	N.E.	---	7
d. oxidation & photolysis to NO _x (stratosphere)	N.E.	---	0.04
e. gaseous deposition	<u>90</u>	<u>74.9</u>	<u>---</u>
TOTAL	440	98.4	17.04

N.E. = Mechanism recognized but no estimate made.

*NOTE: (see note in Table VI)

± Source strength here was adjusted by R. & R. to provide an additional amount of nitrogen needed to balance other portions of their nitrogen compound cycle.

OXIDANTS

OZONE

The problems involved when significant amounts of ozone are present in the atmosphere have come to light probably more as a result of the photochemical pollution problem in Los Angeles than from any other single factor. While background concentrations of ozone probably range from about $20\text{--}60\text{ }\mu\text{g}/\text{m}^3$ ($0.01\text{--}0.03\text{ ppm}$), in urban centers like Los Angeles, it is not unusual to have O_3 present at levels greater than $500\text{ }\mu\text{g}/\text{m}^3$ ($.25\text{ ppm}$). Ozone levels up to $400\text{ }\mu\text{g}/\text{m}^3$ (0.2 ppm) usually will not cause any deleterious effects (Masters, 1971), but at concentrations of $600\text{ }\mu\text{g}/\text{m}^3$ (0.3 ppm) ozone causes irritation of the mucous membranes in the nose and throat. At somewhat higher levels, it can cause coughing, choking and severe fatigue. When present at relatively high levels, such as those that occur in severe photochemical smogs, ozone causes bronchial irritation and interferes with normal lung functioning, causing breathing difficulty and chest pains. For reference sake, the highest ozone concentration detected in the Los Angeles atmosphere was $2,000\text{ }\mu\text{g}/\text{m}^3$ (0.99 ppm) in 1956 (Chambers, 1958, as cited in Tebbens, 1968).

Sources

Because the wavelengths of the ultraviolet radiation that penetrate the troposphere are too long to cause photodissociation of oxygen, it has long been accepted that the presence of ozone in the troposphere is due primarily to the transport of ozone down from the stratosphere. The amount present in the troposphere would then be related to the injection rate through the tropopause, estimated as ranging between 1.9 and $7.5 \times 10^3\text{ kg/yr}$ (Junge, 1962).

Recently, Chameides and Walker (1973) proposed a model wherein both seasonal and diurnal variations in the tropospheric ozone density are assumed to be caused by photochemical changes rather than a change in the flux of stratospheric ozone-rich air into the troposphere. Their model calls for the production of O_3 by the methane oxidation scheme suggested by Crutzen (1973). The oxidation of methane produces hydroperoxyl radicals which react with nitric oxide to form nitrogen dioxide which in turn is photodissociated to NO and O. This atomic oxygen then reacts with O_2 to form ozone.

Removal Mechanisms

Ozone is relatively insoluble in water; at 20°C its solubility is 0.052 g/100g H_2O . Therefore, removal of ozone from the atmosphere by wash-out and rainout can be disregarded. There is evidence though that ozone is removed by the oceans to some extent (Aldaz, 1969). Ozone is also absorbed by vegetation (Hill, 1971; Hill and Littlefield, 1969; and Rich et al., 1970), and soil (Junge, 1962; Kroening and Ney, 1962; Aldaz, 1969; and Turner et al., 1973). Aldaz (1969) has shown that soil and vegetation probably represent a major sink for this gas. He estimated the sink strength of the earth's surface to lie between 1.3 and 2.1×10^{12} kg O_3 /yr.

Due to its nature as a strong oxidizing agent, ozone participates in a number of atmospheric reactions, especially in polluted atmospheres; namely the photooxidation of hydrocarbons in the presence of nitrogen dioxide. The initial oxidation of olefins by ozone, for instance, can lead to a long series of reactions which produce ketones, aldehydes, organic acids and nitrogen-containing compounds such as peroxyacetylnitrate (PAN). The presence of these compounds in the atmosphere has been shown to be the cause of considerable eye irritation (Schuck and Doyle, 1959). Rate constants for the reaction of ozone with numerous hydrocarbons have been

summarized by Altshuller and Bufalini (1971) and Bufalini and Altshuller (1965). Because the reactions of ozone in polluted atmospheres are so numerous and have been the subject of extensive investigation and review, it would not serve the best interest of this paper to review these reactions here. For additional information the reader is referred to Hecht and Seinfeld (1972), Dütsch (1971), Ripperton and Vukovich (1971), Stephens (1969), Altshuller and Bufalini (1965), and Leighton (1961). Junge (1962) has estimated the tropospheric residence time of ozone to range between 3 and 4 months.

HYDROCARBONS

Hydrocarbons constitute a major group of air contaminants which can be subdivided into reactive and non-reactive classes. The more important reactive hydrocarbons include the olefins and aromatics. Paraffinic hydrocarbons are classified as non-reactive.

REACTIVE HYDROCARBONS

Because of their role in photochemical reactions in polluted atmospheres, reactive hydrocarbons have been the subject of great interest. These photochemical reactions produce smog which is associated with eye and respiratory tract irritation, reduced atmospheric visibility, and plant damage.

Limited ambient data from Point Barrow, Alaska (Robinson and Robbins, 1968) indicate that ethylene, the most abundant hydrocarbon of this group, is present at a concentration of less than $1 \mu\text{g}/\text{m}^3$ (less than 1 ppb). In the absence of other ambient measurements one might consider the concentration of ethylene measured at the above location to represent the upper limit of the background concentration for components in this group.

Sources

A variety of hydrocarbons are released to the atmosphere as a result of both anthropogenic activity and natural processes. The most important anthropogenic source of hydrocarbons, resulting from the incomplete combustion of fuel, is motor vehicle exhaust. Robinson and Robbins (1968) estimate that the total annual emission of olefins and aromatics resulting from the combustion of various fuels is 27×10^9 kilograms. A bibliography of various emission sources has been compiled by the U.S. Department of Health, Education and Welfare (1970).

Plant species also release appreciable quantities of volatile organic substances to the surrounding air. The major reactive hydrocarbons emitted by trees are ethylene, monoterpene (C_{10}), and isoprene (C_5). In a recent study, Rasmussen (1972) concluded that the forests represent a global natural source of 175×10^9 kg of reactive hydrocarbons each year. This emission rate is 6 times greater than that estimated for reactive hydrocarbons of anthropogenic origin.

Removal Mechanisms

Hydrocarbons in general are not water soluble, and therefore, they cannot be directly removed from the atmosphere by wet processes such as washout and absorption by surface waters. Various studies have shown that photochemical reactions are important in removing reactive hydrocarbons, although the products formed may cause detrimental side effects such as eye and throat irritation. Hydrocarbons of this class, upon their emission into the atmosphere, undergo rapid chemical transitions in the presence of: atomic oxygen and ozone (Bufalini and Altshuller, 1965); oxides of nitrogen (Shuck, 1961; and Alley *et al.*, 1965); ozone and sulfur dioxide (Cox and Penkett, 1971b) and; nitrogen dioxide and sulfur dioxide (Schuck and Doyle, 1959).

The basic kinetic mechanisms of hydrocarbon reactions in the atmosphere are given by Hecht and Seinfeld (1972). These authors have presented a 15-step mechanism for photochemical smog formation, with rate constants and stoichiometric coefficients chosen according to the particular hydrocarbons involved in the reactions and the initial reactant ratios. The state of the art of photochemical reactions is analyzed by Dodge (1973) and Seinfeld, Hecht and Roth (1973).

Quantitative data on the rates of these atmospheric reactions are rare. The limited data available as reported by Hidy (1973) suggest that 1-10% by weight of the reactive hydrocarbons emitted into the atmosphere are converted to aerosol and eventually are removed by scavenging or deposition. The remaining hydrocarbons are eventually oxidized to carbon dioxide and water vapor.

Smith et al., (1973) investigated the capacity of soils to absorb ethylene and acetylene. They concluded, as did Abeles et al. (1971) in an earlier experiment on ethylene uptake by soil, that the sorption of both ethylene and acetylene is due to microbial activity in the soil. Smith et al. found that the soils they tested removed ethylene at average rates ranging from $.14-.97 \times 10^{-9}$ mol per gram of soil per day (mol/g·d) and acetylene from $.24-3.12 \times 10^{-9}$ mol/g·d.

NON-REACTIVE HYDROCARBONS

This group, which consists of methane and the higher saturated hydrocarbons, has been found to be much less involved in photochemical reactions and smog formation than reactive hydrocarbons. By far the most abundant paraffinic hydrocarbon in the atmosphere is methane. Methane's background concentration is about $1000 \mu\text{g}/\text{m}^3$ (1.5 ppm), while the background concentration for heavier gases in this class is less than $1 \mu\text{g}/\text{m}^3$ (less than 1 ppb) (Robinson and Robbins, 1968).

Sources

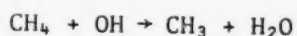
The anthropogenic source of paraffinic hydrocarbons is the incomplete combustion of fuel in motor vehicles. The annual emission of paraffinic hydrocarbons is estimated to be 60×10^9 kilograms (Robinson and Robbins, 1968).

Among natural sources approximately 310×10^9 kilograms of methane

is produced annually in swamps and various water bodies as a result of bacterial decomposition. The relatively high concentration of methane in the atmosphere compared to other organic gases is related to this natural process.

Removal Mechanisms

Because they are so insoluble in water, paraffinic hydrocarbons can not be removed from the atmosphere by wet processes. The primary sink for methane in the troposphere is its oxidation by hydroxyl radicals to form carbon monoxide. The initial reaction is as follows:



The rate coefficient for this equation equals $5.5 \times 10^{-12} \exp(-1900/T)$ (Greiner, 1970). For a complete development of this oxidation scheme the reader is referred to Levy (1971), McConnell *et al.* (1971) and Levy (1972, 1973a). Based upon density profiles of CH_4 and hydroxyl radicals in the troposphere, and the rate equation given above, Levy (1973b) was able to calculate the average daily loss of methane at a particular altitude. The total column loss rate for methane was found to be $7.48 \times 10^{-8} \text{ mol/m}^2 \text{ sec}$. This results in a tropospheric residence time for methane of 2 years.

Rasmussen *et al.* (1968) and Robinson and Robbins (1968) have also suggested that the volatile organic components of the atmosphere are removed by bacteriological processes and vegetation. However, quantitative data and rate equations for these removal mechanisms are nonexistent in the literature.

RECAPITULATION

1. Hydrogen sulfide, sulfur dioxide, nitrous oxide, nitric oxide, nitrogen dioxide, ammonia, carbon monoxide, ozone, and some hydrocarbons have been surveyed regarding their sources and sinks because of their importance as gaseous atmospheric pollutants.

2. In recent years vastly increased information on pollutant sources, sinks, and background levels has become available. Sheer speculation is being replaced by documentation. Still the current state of understanding is changing so fast that there emerge regularly whole new concepts which alter our thinking by orders of magnitude and even in direction.

3. The comprehensive search for natural pollutant removal mechanisms lead to the identification of the following processes: absorption (often accompanied by chemical reaction) by vegetation, soil, water bodies, and natural stone; precipitation scavenging; and chemical reactions in the atmosphere. The relative importance of these processes depends on the particular pollutant and on environmental circumstances. Quantitative modeling of most of these removal processes was found to be in its infancy.

4. For clarity and brevity many details of interest only to a limited audience have been omitted from this article. Such peculiar details as well as extended discussion of conflicts among the available information are presented in a separate report by Rasmussen, Taheri, and Kabel (1974).

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The kind of preliminary quantitative modeling which has been done so far is shown by the following three examples concerning removal of SO_2 from the air at rock and ocean interfaces.

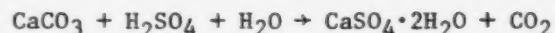
1.3.2. Rock: Living matter has a threshold limit of tolerance to pollutants, below which no injury will occur, and, in fact, the substance might actually benefit from the presence of that pollutant. Rock reacts with pollutants such as SO_2 , at all concentrations. The results of these reactions may not be visible for quite some time, for the effects are cumulative. The extent of breakdown of the rock is therefore less a product of the momentary concentration of the pollutant than the uptake per unit time on a unit area of the material (Luckat, 1973).

The effects of SO_2 on frescoes, monuments and other edifices have been most pronounced over the last century, especially in Europe where high-sulfur coal and oil are used as heating fuels. The basic destructive reaction is that of sulfuric acid ($\text{SO}_2 + 1/2 \text{O}_2 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{SO}_4$) on the carbonate matrix of limestone and sandstone in the presence of moisture. Spedding (1969) has shown that as the relative humidity in the air increases, the SO_2 uptake rate by oolitic limestone increases significantly (Table I).

Table I. UPTAKE OF SO_2 BY OOLITIC LIMESTONE

Relative Humidity %	SO_2 concentration $\mu\text{g}/\text{m}^3$	Time of exposure min.	Uptake $\mu\text{g SO}_2/\text{cm}^2$ of surface	Uptake rate $\mu\text{g}/\text{cm}^2 \cdot \text{d}$
11	360	20	0.069	5.0
13	280	40	0.061	2.2
79	100	48	0.24	7.2
81	370	10	0.28	40.3

The product of the reaction between sulfuric acid and the carbonate matrix is gypsum if sufficient evaporation occurs:



Because the calcium carbonate is slowly being replaced by gypsum, the rock would be subject to increased weathering rates due to:

- (1) an enhanced chemical disintegration caused by the much greater solubility of gypsum in water than calcium carbonate. The newly formed mineral would be subject to dissolution in water with accompanied leaching out of the rock, and
- (2) an enhanced physical disintegration caused by the almost two-fold volume expansion in the rock accompanying the formation of gypsum.

Other properties such as the density and porosity of the rock are also important and affect the amount of weathering to be expected in a rock per unit uptake rate; a rough, porous, lime-cemented sandstone would be expected to weather faster than a smooth, dense limestone (Luckat, 1973).

To determine whether the absorption of SO_2 by sedimentary rocks would constitute a significant sink for SO_2 , a number of assumptions were made:

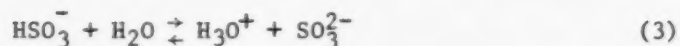
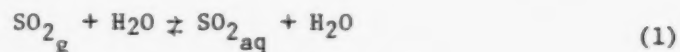
- (1) Knowing that approximately 30% of the total earth's surface area of about $5 \times 10^{14} \text{ m}^2$ was land (Holmes, 1965), and assuming that perhaps 5% of the land surface had exposed rock (F. E. Wickman, 1974), and of this approximately 75% is sedimentary (Leet and Judson, 1965), it was calculated that about 1% of the total earth's surface was covered with rock capable of absorbing SO_2 .

- (2) Luckat (1973) and Spedding (1969) found SO_2 absorption rates ranging from 5-200 $\text{mg/m}^2\cdot\text{d}$ in sandstone and limestone, respectively. Luckat's measurements were taken in a highly industrialized region of Germany; Spedding's measurements were made with SO_2 concentrations approximately 100 times greater than the average world-wide background concentration. For this calculation, the lower limit of 5 $\text{mg/m}^2\cdot\text{d}$ was used.

From these values it was calculated that approximately 9×10^9 kg SO_2/yr or 4.5×10^9 kg S/yr could be removed by stone under these optimal and exaggerated conditions. Comparison of this value with those in Table IV of the paper included earlier in this report shows this value to be considerably smaller than that of any other natural SO_2 sink.

There are many problems related with making any such estimate as was done above. First of all, any estimate of the total percentage of the earth's surface which has exposed rock is entirely speculative at this time because geological maps are not available for all parts of the world. Then again, there is the problem of defining an outcrop and mapping it in its strictest sense; that is, mapping the outcrop without magnification and without the inclusion of soils or detritus as part of the outcrop. There is also the fact that not all the sedimentary rock that is exposed is sandstone or limestone; much of it is shale or mudstone or something of similar density which would probably not absorb SO_2 to any extent. Finally, the areas where most of the rock does outcrop would be in areas where the SO_2 level would probably be quite low. It can therefore be assumed that rock constitutes a negligible sink for SO_2 on a global scale.

1.3.3. SO₂ Solubility: Most data on SO₂ solubility in the literature have been determined when atmospheric SO₂ concentrations in the experimental chambers far exceeded those found in ambient air. Hales and Sutter (1973) worked towards closing this obvious gap by running a number of experiments to help "quantify the relationships between SO₂ solubility, concentration, and hydrogen-ion impurity at levels normally encountered in nature." The dissolution of SO₂ was assumed to proceed according to the reactions set forth by Falk and Giguere (1958):



The second ionization (reaction 3) was assumed to be negligible.

Based upon the first two of the above reactions, Hales and Sutter derived an "extrapolation equation, relating the concentration of total dissolved SO₂ in water (C_{SO₂}) to airborne concentration and solution acidity" as follows:

$$\begin{aligned} C_{\text{SO}_2} &= [\text{SO}_2]_{\text{aq}} + [\text{HSO}_3^-] \\ &= \frac{[\text{SO}_2]_g}{H} + \frac{-[\text{H}_3\text{O}^+]_{\text{ex}} + \sqrt{[\text{H}_3\text{O}^+]_{\text{ex}}^2 + 4 K_1 [\text{SO}_2]_g / H}}{2} \quad (4) \end{aligned}$$

where those terms bracketed are concentrations in moles per liter and $[\text{H}_3\text{O}^+]_{\text{ex}}$ is the "excess" hydrogen ion concentration, defined as the concentration of hydrogen ion in solution present due to sources other

than the dissolving of SO_2 . K_1 is the equilibrium constant for reaction (2) and H is the Henry's law constant. Extrapolation of SO_2 solubility data from Johnstone and Leppla (1934) down to low ambient SO_2 concentrations show deviations ranging from 0.7 to 21.2% of those by Hales and Sutter. In general, the percent deviation increased as the concentration of SO_2 in the gas phase decreased. The authors suggest that even though this deviation does exist, the ability of equation (4) to predict low SO_2 concentration solubility appears excellent and they recommend its use whenever low concentration solubility data are needed.

A more exact equation for determining the total dissolved SO_2 in water can be derived based on the solution equilibria involved. The resulting equation not only takes into consideration the pH of the solution and the atmospheric partial pressure of the gas, P_{SO_2} , but applies to different aqueous phase conditions, including both sea water and rain water. Also, it eliminates the use of the often confusing and now outdated hydronium ion (H_3O^+). The dissolution and dissociation reactions for SO_2 in water are more correctly written (Scott and McCarthy, 1967)



In the equations which follow the activity, a , of the aqueous species is denoted by brackets []. The activity and the molality of a species are related by the activity coefficient, $a = m\gamma$. In dilute solutions the molality (moles/1000g H_2O) of a species is approximately equal to its molarity (moles/l H_2O). Rigorously the activity is dimensionless but for calculational purposes it may be taken to have the dimensions of molality or molarity with the activity coefficient being dimensionless.

Johnstone and Leppla (1934) and Scott (1964) show that reaction (5) follows Henry's law for dilute solutions up to concentrations of at least one molar. Thus,

$$H = \frac{[SO_2 \cdot H_2O]}{P_{SO_2}} \quad (8)$$

where $[SO_2 \cdot H_2O]$ is the activity of solvated sulfur dioxide and P_{SO_2} is the SO_2 partial pressure in atmospheres. The defining equations for the ionization constants are:

$$K_1 = \frac{[H^+][HSO_3^-]}{[SO_2 \cdot H_2O]} \quad (9)$$

$$K_2 = \frac{[H^+][SO_3^{--}]}{[HSO_3^-]} \quad (10)$$

Using equations (8), (9), and (10), a molal mass balance for the system can be written

$$\Sigma m_{\text{SO}_2} = m_{\text{SO}_{2\text{aq}}} + m_{\text{HSO}_3^-} + m_{\text{SO}_3^{=}} \quad (11)$$

wherein,

$$m_{\text{SO}_{2\text{aq}}} = \frac{H^{\text{P}}_{\text{SO}_2}}{\gamma_{\text{SO}_{2\text{aq}}}} \quad (12)$$

$$m_{\text{HSO}_3^-} = \frac{K_1 H^{\text{P}}_{\text{SO}_2}}{\gamma_{\text{HSO}_3^-} [\text{H}^+]} \quad \text{and} \quad (13)$$

$$m_{\text{SO}_3^{=}} = \frac{K_2 K_1 H^{\text{P}}_{\text{SO}_2}}{\gamma_{\text{SO}_3^{=}} [\text{H}^+]^2} \quad (14)$$

Substituting the values for the molality for each of these species into equation (11), the following general formula for the concentration of dissolved SO_2 is derived:

$$\Sigma m_{\text{SO}_2} = H P_{\text{SO}_2} \left(1/\gamma_{\text{SO}_2\text{aq}} + K_1/\gamma_{\text{HSO}_3^-} [\text{H}^+] + K_2 K_1/\gamma_{\text{SO}_3^{2-}} [\text{H}^+]^2 \right) \quad (15)$$

The definition of pH is

$$\text{pH} = -\log [\text{H}^+]$$

Therefore, by convention, in equations the activity of the hydrogen ion can be written $[\text{H}^+] = 10^{-\text{pH}}$ as desired.

For use in predicting SO_2 solubility, equation (15) requires values for H , K_1 , K_2 and the three activity coefficients in addition to the pH and the SO_2 partial pressure. Scott and Hobbs (1967) give $H = 1.24$, $K_1 = 0.0127$, and $K_2 = 6.24 \times 10^{-8}$ at 25°C . Corresponding data at other temperatures are given by Johnstone and Leppla (1934). One case of considerable interest is the absorption of SO_2 in sea water. Activity coefficients of aqueous sulfite species, $\text{SO}_2 \cdot \text{H}_2\text{O}$, HSO_3^- , and SO_3^{2-} in sea water are not available. However, Reardon (1974) determined activity coefficients for the analogous carbonate species and also sulfate ion in sea water. From a point of view of similarity of species and coherence among the variables, the sulfate activity coefficient is rejected in favor of use of the carbonate species activity coefficients. Hence,

$$\gamma_{\text{SO}_2\text{aq}} \approx \gamma_{\text{H}_2\text{CO}_3^0} = 1.19$$

$$\gamma_{\text{HSO}_3^-} \approx \gamma_{\text{HCO}_3^-} = 0.67$$

$$\gamma_{\text{SO}_3^{2-}} \approx \gamma_{\text{CO}_3^{2-}} = 0.19$$

By substituting these values into equation (15), and assuming that sea water has a pH of 8.1, equation (15) reduces to

$$\Sigma m_{\text{SO}_2} = 8.42 \times 10^7 P_{\text{SO}_2} \quad (16)$$

where the amount of dissolved SO_2 is seen to be a linear function of the atmospheric partial pressure of SO_2 .

The minimum background concentration of SO_2 is $1 \mu\text{g}/\text{m}^3$ which corresponds to 3.8×10^{-10} atmospheres SO_2 partial pressure. From equation (16) the amount of SO_2 dissolved in sea water at equilibrium would be 3.2×10^{-2} mol/l. As an upper limit one might consider ambient SO_2 concentrations found by Luckat (1973) in highly industrialized sections of Germany. The observed $360 \mu\text{g}/\text{m}^3$ is equivalent to $P_{\text{SO}_2} = 1.4 \times 10^{-7}$ atm. In equilibrium with such an atmosphere sea water would absorb 11.6 mol SO_2 /l. This molarity is an order of magnitude higher than that where Henry's law is known to hold. Thus, the predictive equation might fail under these circumstances.

When the dissolution of SO_2 takes place in rain water, the activity coefficients required for equation (15) may be assumed equal to unity because the ionic strength of rain water (a measure of the interionic effect resulting primarily from electrical attraction and repulsions between the various ions) would be very low, probably on the order of 10^{-4} . Therefore, equation (15) reduces to

$$\Sigma m_{\text{SO}_2} = P_{\text{SO}_2} \left(1.24 + \frac{1.58 \times 10^{-2}}{[\text{H}^+]} + \frac{9.83 \times 10^{-10}}{[\text{H}^+]^2} \right) \quad (17)$$

In this case the hydrogen ion activity is dependent upon the amount of SO_2 absorbed and cannot be specified a priori. The charge balance for the dissolution and dissociation reactions of SO_2 in water is

$$[\text{H}^+] = [\text{HSO}_3^-] + 2[\text{SO}_3^{--}] + [\text{OH}^-]$$

By substituting in the respective expressions for the $[\text{HSO}_3^-]$ and $[\text{SO}_3^{--}]$ as given by equations (8, 9, and 10), and setting $[\text{OH}^-] = 10^{-14}/[\text{H}^+]$, an expression is derived for the partial pressure of SO_2 as a function of $[\text{H}^+]$ as follows:

$$P_{\text{SO}_2} = \frac{[\text{H}^+]^3 - 10^{-14} [\text{H}^+]}{1.58 \times 10^{-2} [\text{H}^+] + 1.97 \times 10^{-9}} \quad (18)$$

Choosing an initial value for the $[\text{H}^+]$, and substituting that value into equation (18), a corresponding value for P_{SO_2} (atm) can be found. These values for P_{SO_2} and $[\text{H}^+]$ are then in turn substituted into equation (17) to find the amount of total dissolved SO_2 .

In pure rain water the pH is 7.0. Any SO_2 which dissolves would produce an acid solution and a drop in pH. Thus, for pH = 7, $P_{\text{SO}_2} = \Sigma m_{\text{SO}_2} = 0$. For a pH of 5, P_{SO_2} and Σm_{SO_2} are calculated to be 6.3×10^{-9} atm and 1.0×10^{-5} mol/l, respectively. For a pH of 3, $P_{\text{SO}_2} = 6.35 \times 10^{-5}$ atm and $\Sigma m_{\text{SO}_2} = 1.1 \times 10^{-3}$ mol/l. Clearly as P_{SO_2} increases, the amount of dissolved SO_2 increases and the pH decreases. The dissolved SO_2 predicted by equations (17) and (18) agree excellently with the experimental data of Hales and Sutter (1973) and Terraglio and Mangarelli (1967).

1.3.4. Rate of SO₂ absorption by sea water: The solubility of SO₂ in sea water as discussed in the preceding paragraphs is only the equilibrium limit of the absorption process. It is much more complex to quantitatively model the rate of absorption. A parameter commonly used in such quantification is the deposition velocity. Kabel (1973) showed the relation between the deposition velocity, v_D , and the mass transfer coefficient, k_g . He showed how a simple extension of the Reynolds analogy could be used with a boundary layer characterization of the fluid mechanics to predict the deposition velocity for ammonia absorption. The following example illustrates a somewhat different approach which is carried through to the determination of the distance polluted air must travel over the ocean to have a specified proportion of the SO₂ removed. It should be kept in mind in following this example that many alternative models and assumptions are possible.

For correlation of mass and momentum transfer, Perry, et. al. (1963) give

$$k_g = \frac{f}{2} \frac{\bar{v} \rho}{Sc^{2/3}} \quad (19)$$

where f is the friction factor, $\bar{v}$ is the average velocity, ρ is the inert component mass density, and Sc is the Schmidt number. For flat surfaces the friction factor can be estimated from various correlations (Schlichting, 1968; Sherwood, 1950; Schnautz, 1958). However, perhaps the most promising and applicable route to the friction factor

is via models which predict wind velocity profiles over various surfaces. One such well established model, for an adiabatic lapse rate, is (Pasquill, 1962)

$$\frac{v}{v_*} = \frac{1}{k} \ln \frac{z}{z_0} \quad (20)$$

where v_* is the friction or shear velocity, v the wind velocity at height z , and z_0 is a roughness length characteristic of the ground surface (for smooth sea Schnautz (1958) gives $z_0 \approx 2 \times 10^{-4}$ m). Von Karman's constant k is taken to be 0.4. The friction velocity is related to the ground level shear stress, τ_0 , by (Sutton, 1949)

$$v_*^2 = \frac{\tau_0}{\rho} = \frac{f}{2} \bar{v}^2 \quad (21)$$

The friction velocity can be obtained from equation (20) by measuring the velocity v_1 at height z_1 . With v_* known, equation (20) provides the velocity profile which can be integrated over the range of height, $z=0$ to $z=H$, to give the average velocity as

$$\bar{v} = \frac{\int_0^H v dz}{\int_0^H dz} = \frac{\int_0^H \frac{v_*}{k} \ln \frac{z}{z_0} dz}{H} \quad (22)$$

Knowing $\bar{v}$ the friction factor can be obtained from equation (21) and equation (19) can be solved directly for k_G .

The removal of SO_2 from air, $Sc=1.28$ at 0°C , 1 atm (McCabe and Smith, 1967), over a natural surface such as sea water can now be estimated. For the case of $v_1 = 5\text{ m/s}$ at $z_1 = 2\text{ m}$, v_* is found to be 0.216 m/s and $\bar{v}$ (up to an inversion height of 100 m) = 6.6 m/s . Scorer (1968) discusses inversion heights for a variety of cases. The friction factor is then 0.00228 and k_G is $7.53\text{ g/m}^2\text{ s}$. For a very small equilibrium vapor pressure of SO_2 over sea water, the deposition velocity can be calculated from the mass transfer coefficient by dividing k_G by the air density, hence $v_D = k_G / \rho_{\text{air}} = 0.64\text{ cm/s}$. This result is comparable in magnitude to literature values.

Now one can crudely estimate the effects of this removal mechanism downstream of a line source of the pollutant. Neglecting end effects and assuming that all fluid motion is between ground level and an inversion height of 100 m and that the logarithmic velocity profile is adequate, the rate of mass transfer per unit length of source can be expressed by a mass balance about an element of height, H , and thickness, dx , as

$$H\bar{v}dC = v_D C dx \quad (23)$$

where x is the distance downwind of the line source. The boundary condition is $C(x=0) = C_0$. Solving equation (23) leads to

$$\ln \frac{C(x)}{C_0} = \frac{v_D x}{\bar{v}H} = 9.65 \times 10^{-6} x \quad (24)$$

From equation (24) one can calculate that 90 and 99% of the SO_2 would be removed at downstream distances of 238 and 476 km, respectively. It might be noted that the height H strongly affects the distance required to remove a fixed proportion of the pollutant; however, values of $\bar{v}$, f , v_D , etc. are little changed.

The foregoing analysis is based on several simplifying assumptions. First, it is assumed that the logarithmic velocity profile is valid. This assumes that an adiabatic lapse rate exists, an assumption inconsistent with those used in the calculation of concentration downwind of a line source under an inversion. Note that the complete air pollution meteorology model should provide a velocity profile and this contradiction will not occur.

To allow for the fact that the zero velocity may occur at a point other than the actual earth interface, this equation can be modified. For example, z can be replaced by $z+d_0$ where d_0 is a displacement factor to designate the point of zero velocity. However, for transfer to sea water $d_0 \ll z$. There is also some uncertainty in the estimate of the roughness length over water. It is also assumed that the velocity profile is unchanged downwind of the source.

Another assumption made is that the Reynolds analogy holds and that the molecular dispersion of pollutants is negligible. It was further assumed that the equilibrium vapor pressure of the pollutant at the ocean interface is very small at all times (i.e. the sea is a perfect sink). This restriction is readily removed by use of the SO_2 solubility correlation presented earlier. And the SO_2 concentration

is taken to be uniform in the vertical direction. In the line source calculation, the assumption was made that all unabsorbed pollutant was held between the sea and the arbitrarily chosen inversion height. Many of these assumptions are arbitrary and can be varied at will.

It is possible to approach the problem of mass transfer at the interface differently. One could deal with dispersion coefficients instead of mass transfer coefficients. In this case the rate of removal would be expressed in terms of the dispersion coefficient and concentration gradients. The dispersion coefficient can be obtained from the velocity profile information. Such an approach will be considered in further work.

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V OBSERVING SYSTEMS FOR URBAN AND REGIONAL ENVIRONMENTS

Part 1

INTERPRETATION OF ACDAR SOUNDING OBSERVATIONS

OBSERVING SYSTEMS FOR URBAN AND REGIONAL ENVIRONMENTS

Preface

Measurements-oriented research activities within the SRG are included in both the Department of Meteorology (DM) and Center for Air Environment Studies (CAES). Within the DM, studies are concentrated in two specific problem areas. They are, as defined in the scope of work in the original SRG proposal (18.1.72), to:

a) Task 1D

"Perform studies relating to the comparative applicability of various remote sensing instrumentation systems for economically providing the data required for evaluating and applying numerical air pollution simulation models".

and

b) Task 4

"Modify the PSU aircraft for use in air pollution field measurements needed for providing initial conditions for numerical models and for verifying them. Particular emphasis will be placed on the installation and testing of equipment for gaseous and particulate air pollution sampling."

For air pollution and urban-to-mesoscale meteorology related measurements, acdar and lidar systems continue to yield some of the most dramatic and useful observations of atmospheric structure and dynamics, and aerosol, respectively. The wider (and more quantitative) application of acdar systems depends upon "theoretical-physical" research regarding techniques for processing and interpreting the received acdar signals. This has been the focus of research conducted by members of Task Group 1D.

In particular, the research to date has been concerned with numerical simulation of received signals and analysis of the capabilities and limitations of acdar systems (of many different configurations) for tropospheric temperature, wind profile and turbulence measurements. To the extent required for checking theoretical work in progress, experimental acdar systems have been developed and used in field measurements at Penn State.

Rather than undertake theoretical studies, such as that of the well known "inversion" problem regarding the interpretation of lidar data, we noted the lack of suitable airborne systems for obtaining direct measurements of atmospheric aerosol at heights greater than those of instrumented towers. Consequently, the research effort related to the evaluation of lidar systems has for all practical purposes been integrated into Task 4. That is, we have undertaken and have, now, nearly completed the development of a comprehensive airborne instrumentation package capable of obtaining direct aerosol measurements in the regions probed by existing lidar systems. Thus, during cooperative aircraft-lidar experiments, we have a unique capability for obtaining data for direct-indirect intercomparison studies.

Under the auspices of the SRG grant, in Task Group 4 we have developed, and used for a variety of experiments, what is probably the most comprehensive university-based airborne meteorological and aerosol instrumentation system in the world. A complement of nearly 40 individual sensors and instruments output data from which diverse meteorological, turbulence, aerosol, and radiation quantities are derived. Extraordinary

care has been taken in, for example, designing and fabricating the isokinetic sampling tube and radiometer mounts to insure that data will be non-biased and have the highest possible signal/noise ratio.

Only recently completed, the reconfigured aircraft has not only been extensively used for individual SRG in-house research studies, but also been flown more than 100 hours in conjunction with other EPA measurement programs in the St. Louis Regional Air Pollution Study (RAPS).

The following pages summarize some of the individual efforts which have contributed to the overall progress made by Task Groups 1D and 4.

1.0 TASK 1D-INTERPRETATION OF ACDAR SOUNDING OBSERVATIONS

1.1 Introduction

A propagating pulse of acoustic energy emitted by an acdar transmitter is refracted by "average" spatial gradients of temperature and wind and scattered by local turbulent velocity and temperature fluctuations. One may choose to measure the received power, $P(r)$, as a function of range which may be related to the acoustic refractive index structure functions, C_T^2 and C_V^2 or the signal Doppler shift f_d which may be related to mean and turbulent atmospheric motions.

In their fundamental form the defining equations appear deceptively simple.

$$P(r) = P_o \frac{A_c}{A_T} \frac{A_r}{R^2} L_v \cdot e^{-\int_{\text{Trans.}}^{\text{Scat.}} \alpha(r) dr} \cdot \beta(\theta, r) \cdot e^{-\int_{\text{Scat.}}^{\text{Rec.}} \alpha(r) dr} \quad (1)$$

where P_o = peak transmitted power

A_c = area common to transmitter and receiver beams

A_T = area of transmit antenna

A_r = area of receiver antenna

R = range along L

L_v = length of scattering volume to space

$\alpha(r)$ = extinction coefficient

$\beta(\theta, r)$ = scattering angle dependent volume scatter coefficient

The Doppler spectrum $S(f)$ is given by

$$S(f) df = G(\alpha, \phi) W(\phi) d\alpha \quad (2)$$

where $G(\alpha, \phi)$ is related to the distribution of energy within the antenna beams and the antenna pointing angle, and $W(\phi)$ is the scattering angle dependent volume scatter coefficient, $B(0, r)$, expressed in terms of the antenna pointing angle. But in practice quantitative evaluation of the equations is difficult due to the complicated terms which are used to parameterize the system geometry and atmospheric conditions. Furthermore, it is clearly quite a different problem to evaluate $P(r)$ given all the terms on the right hand side of equation (1) than $\alpha(r)$, and $B(0, r)$ given a series of $P(r)$ measurements. Precise determination of atmospheric motions is also difficult since the observed Doppler spectrum depends upon the integral of combined atmospheric and system dependent functions.

Clearly, if acdar systems are ever to be used on an operational basis for inputting, for example, vector wind and intensity of turbulence as a function of height data into a running regional or urban-scale predictive model, schemes for objectively, and automatically, processing the return signals will be essential. The data reduction procedure currently used by most acdar research groups involves post-experiment subjective-objective evaluation of vertical time sections generated using a facsimile to identify structural features and, if Doppler data is available, analysis of computed spectra to estimate winds.

It is our (Task Group 1D) thesis that if we can precisely define the acdar "system" functions for any specified operating sounder, and adequately model the refraction and scattering of acdar signals in the atmosphere, many experiments which are critical to improving our understanding of acdar measurements can be performed using a numerical simulator in which the system parameters and the atmospheric conditions (the independent variables) can be precisely controlled.

Thus, one aspect of the theoretical work in the group consists, basically, of the analysis of the acdar and Doppler equations. The magnitude of the power and the characteristics of the Doppler spectrum as a function of range as they depend upon both the properties of the sounding system and the highly variable physical state of the atmosphere are being quantitatively dissected and modeled.

A second area of theoretical study concerns the analysis of refractive propagation of sound in surface-based and elevated temperature inversions. When such inversions exist it is, at least theoretically, possible to infer the temperature gradient up to the top of the inversion by using sound refractively propagated over an ≈ 3 to 20 km path. We are presently attempting to establish, using our own field measurements, the utility of the technique.

In general, experimental work by the group has been limited to that minimally necessary to check the theoretical work in progress. One section of this report summarizes field measurements currently underway.

The last section consists of copies of two papers submitted by members of the group to the Journal of Geophysics Research during the past year. Both papers have been accepted for publication, presumably in late 1974.

2.0 ANALYSIS OF DOPPLER-SHIFTED MONOSTATIC ACDAR SIGNALS

R. L. Coulter, Ph.D. Research in Progress

2.1 System Geometry

In any monostatic indirect sensing system, the basic geometry is as described in Fig. (1), where $\phi \equiv$ elevation angle, $\beta \equiv$ azimuth angle and $R \equiv$ distance from the transmitter-receiver to the target.

Generally, a target will have motion along all three perpendicular axes, but for a monostatic system and Doppler frequency shift considerations, the only velocity that really matters is the radial velocity, i.e.

$$V_R = v_x \sin \beta \cos \phi - v_y \cos \beta \cos \phi - v_z \sin \phi$$

But

$$\sin \beta = \frac{x}{R \cos \phi}, \quad \cos \beta = \frac{y}{R \cos \phi} \quad ; \quad \sin \alpha = \frac{z}{R}$$

Thus

$$V_R = \left\{ \frac{xv_x}{R} + \frac{yv_y}{R} + \frac{zv_z}{R} \right\}$$

where the coordinates of the scatterer are (x,y,z) .

To a high degree of accuracy, the Doppler shift due to a scatterer in motion is given by

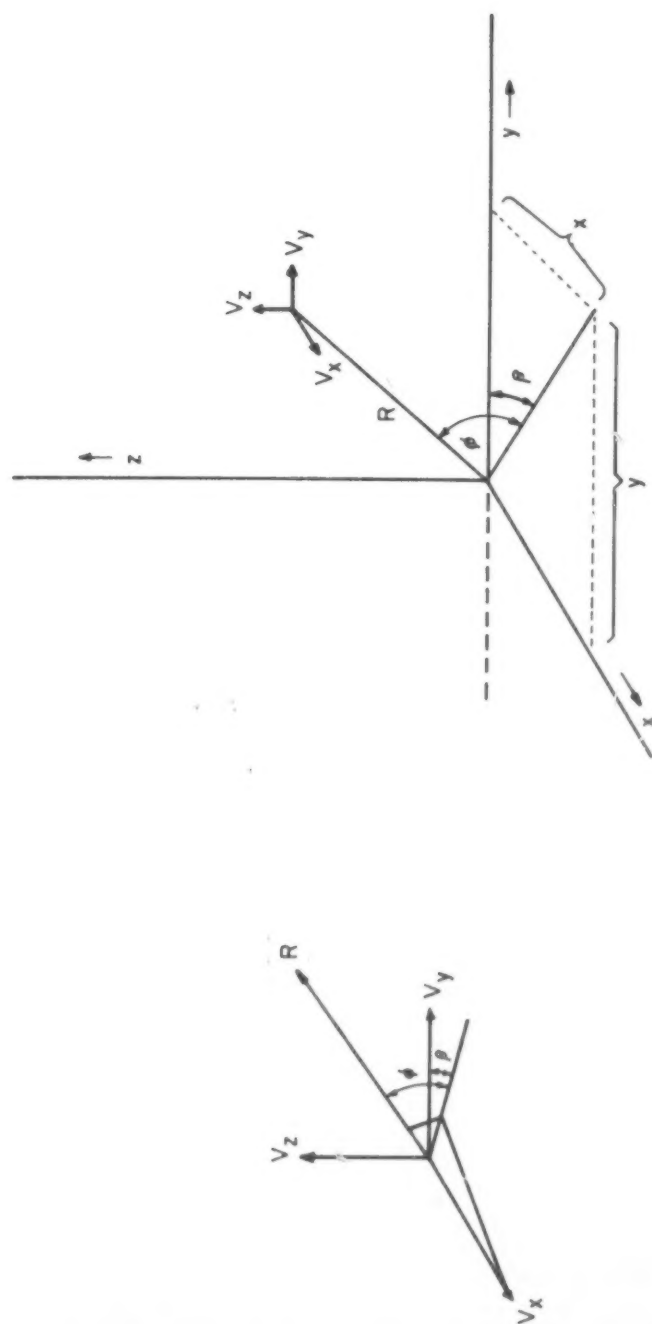


FIGURE 1 : ILLUSTRATION OF COORDINATE SYSTEM AND BASIC ANGLES USED IN TEXT.

$$f_D = \frac{-2V_R}{\lambda} = -\frac{2}{\lambda R} (x v_x + y v_y + z v_z)$$

$$= -\frac{2}{\lambda} \left(\frac{x v_x + y v_y + z v_z}{(x^2 + y^2 + z^2)^{1/2}} \right)$$

If there is an integer number of wavelengths between transmitter and target, we can determine the equiphase geometry by

$$2R = n\lambda \Rightarrow 4(x^2 + y^2 + z^2) = (n\lambda)^2$$

$$(x^2 + y^2 + z^2) = \left(\frac{n\lambda}{2}\right)^2$$

i.e., the equiphase surfaces, disregarding phase velocity changes with wind speed and/or temperature structure are a series of concentric spheres of radius $\frac{n\lambda}{2}$.

The normal to the equiphase surfaces in the y-z plane is given by z/y, i.e., any st. line from the center through a point is the normal. Thus, when the wind is along the normal, we have a maximum doppler shift:

$$\frac{v_z}{v_y} = \frac{z}{y}$$

seen in the x-y plane as

$$\frac{v_y}{v_x} = \frac{y}{x}$$

and in the x-z plane as

$$\frac{v_x}{v_z} = \frac{x}{z}$$

2.2 Surfaces of Constant Doppler Shift

In order to evaluate the spectral broadening due to different scatterers within a transmitted beam, a weighting function must be devised which accounts for different scatterers producing the same Doppler shift. Thus, in order to determine this weighting, we must determine the surfaces in space with constant Doppler shift (CODOSS).

First, assume $v_y = 0 = v_z$ and we are at $z = 0$, looking at the x-y plane. In this case, for $f_D = \text{constant}$ we have

$$f_D = - \frac{2x v_x}{\lambda R} = - \frac{2v_x}{\lambda} \frac{x}{(x^2 + y^2)^{1/2}}$$

$$x^2 + y^2 = \frac{4 v_x^2}{x^2 f_D^2} x^2$$

and

$$x = \pm y \left(\frac{1}{\frac{2 v_x^2}{\lambda^2 f_D^2} - 1} \right)^{1/2} \equiv \pm \frac{y}{a}; \quad a^2 \equiv \left(\frac{2 v_x}{\lambda f_D} \right)^2 - 1$$

i.e., at $z = 0$ we have straight lines of slope $\frac{dx}{dy} = \frac{1}{a}$ (Fig. 2).

Of course $z = 0$ is not of interest, so we set $z = z_0$. Now:

$$f_D = - \frac{2x v_x}{\lambda (x^2 + y^2 + z_0^2)^{1/2}}$$

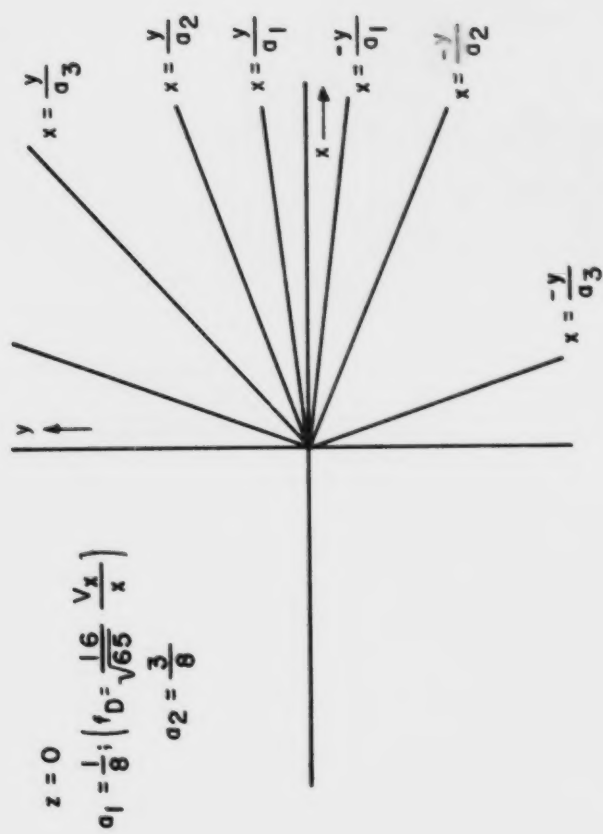


FIGURE 2: LINES OF CONSTANT f_D WHEN $z = 0$.

$$x^2 + y^2 + z_o^2 = \frac{4 v_x^2}{\lambda^2 f_D^2} x^2 + x^2 = \frac{y^2}{a^2} + \frac{z_o^2}{a^2}$$

or

$$\frac{a^2 x^2}{z_o^2} - \frac{y^2}{z_o^2} = 1$$

which is the equation for a hyperbola of asymptote $x = \pm \frac{y}{a}$ and intersection with the x axis ($y = 0$) at $x = \pm \frac{z_o}{a}$ (Fig. 3).

Thus, when $y \gg z$ we tend to straight lines, and when $y \lesssim z$ the surfaces at a height z are sharply curved. In three dimensions, this appears as in Fig. 4 for a given f_D , λ , and $v_y = v_z = 0$.

Similar results hold for $v_x = v_z = 0$ and $v_y = v_x = 0$, except that the hyperbolas are rotated 90 degrees. That is, when there is vertical motion only, the hyperbolas are around the vertical axis with asymptote $z = \pm \frac{x}{a}$. At a constant $z = z_o$ with vertical motion only we have

$$z_o^2 = \frac{x^2}{a^2} + \frac{y^2}{a^2} \quad \text{where now} \quad a^2 = \left(\frac{2 v_z}{\lambda f_D} \right)^2 - 1$$

i.e., in the x, y plane we have a circle of radius a z_o . (Fig. 5)

When v_x and v_y are both non-zero, the same hyperbolas are obtained by rotating the axes through an angle

$$\Theta = \tan^{-1} \frac{v_y}{v_x}$$

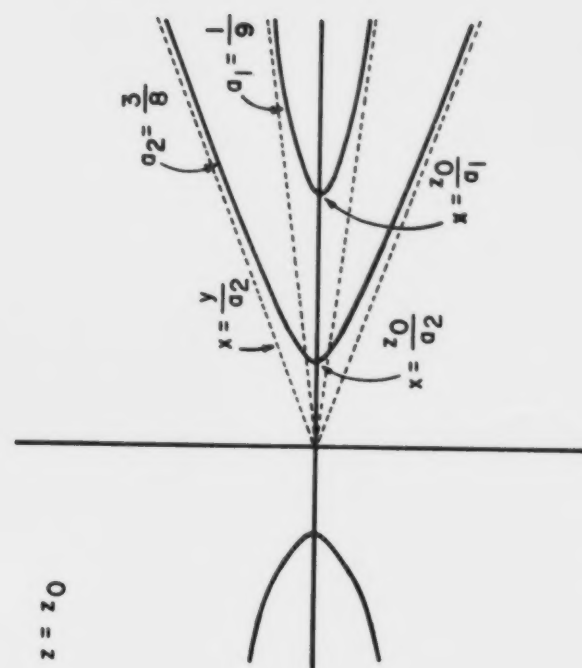


FIGURE 3: WHEN $z = 0$, LINES ARE HYPERBOLAS
WITH $z = 0$ LINES AS ASYMPTOTES.

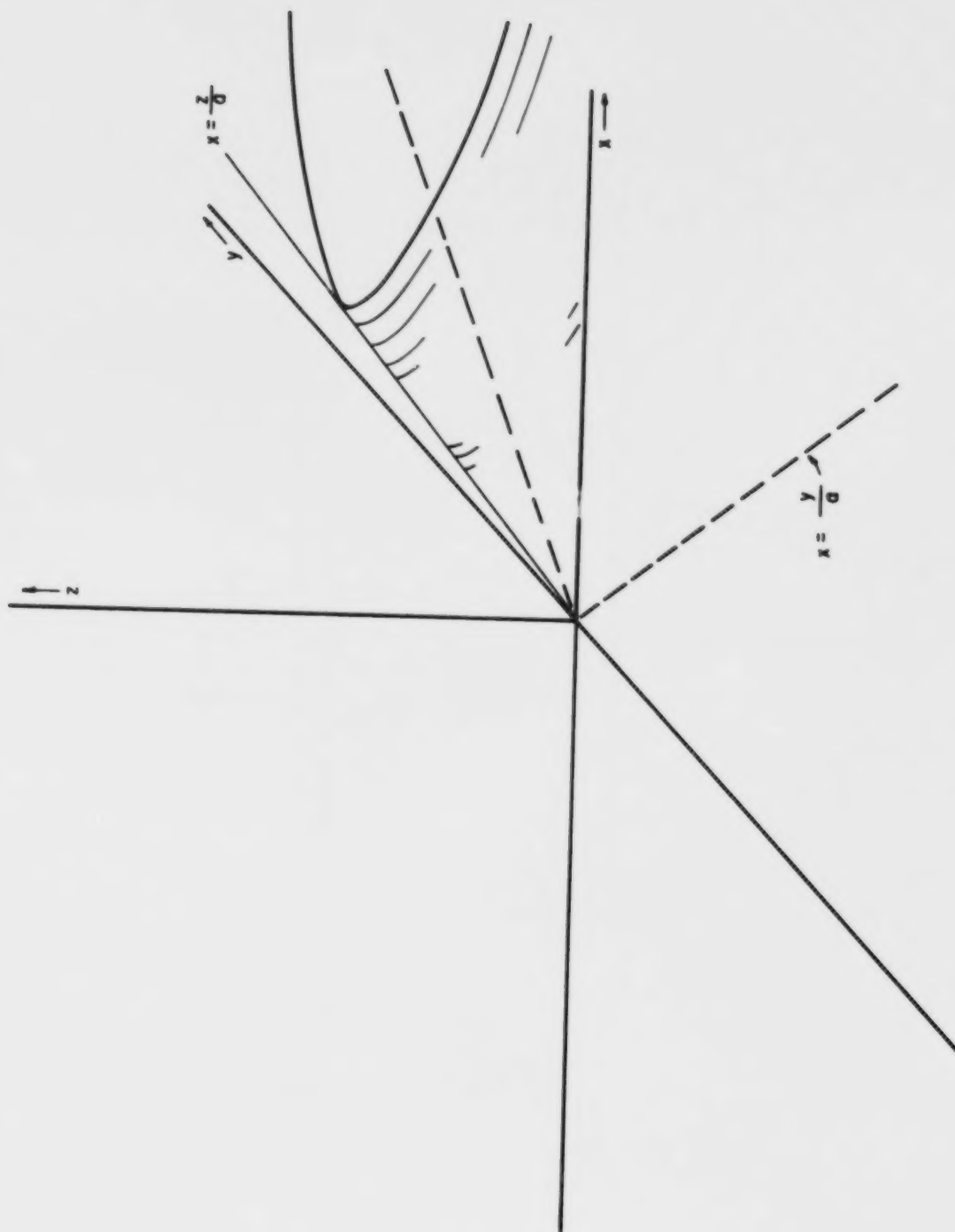


FIGURE 4: THREE DIMENSIONAL DEPICTION OF LINES OF CONSTANT DOPPLER SHIFT WITH HORIZONTAL WIND.

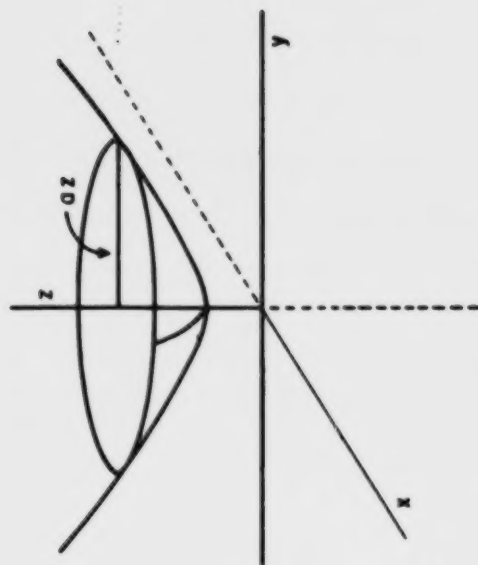


**FIGURE 5: CONSTANT DOPPLER SURFACE FOR
VERTICALLY POINTING SOUNDER WITH
VERTICAL WIND.**

And, if $v_w \neq 0$, after rotating through Θ , rotating through a vertical angle, $\phi = \tan^{-1} \frac{v_z}{v_x}$ will again bring the form back to that of a hyperbola in a plane tilted at ϕ to the horizontal. (Appendix I)

2.3 Horizontal Wind

For simplicity, align the x axis with the horizontal wind. As shown above, no generality is lost. First, consider a transmitter-receiver pointing vertically (Fig. 6). Since the x intercept at any height x is given by $x = \pm z/a$ (the minus sign applicable to the negative shifts which are symmetric in this case to the positive ones), the straight lines (in the $y = 0$ plane) $x = z/a$ determine the closest point at any height z that any given CODOSS comes to the axis of the transmit beam. We can, therefore, determine the maximum and minimum shift for this situation simply by setting this slope equal to the slope of the edge of the conical beam

$$\left. \frac{dz}{dx} \right|_{\text{surface}} = a = \cot \alpha \quad (\alpha = \text{beam width})$$

$$\frac{4v^2}{\lambda^2 f^2} - 1 = \cot^2 \alpha$$

$$f_{\max} = \frac{2v}{\lambda} \left(\frac{1}{1 + \cot^2 \alpha} \right)^{1/2} = \frac{2v}{\lambda} \left(\frac{1}{\frac{\cos^2}{\sin^2} + 1} \right)^{1/2} = \frac{2v}{\lambda} \sin \alpha$$

which is precisely what is to be expected from a scatterer at the edge of the beam and moving horizontally toward the axis.

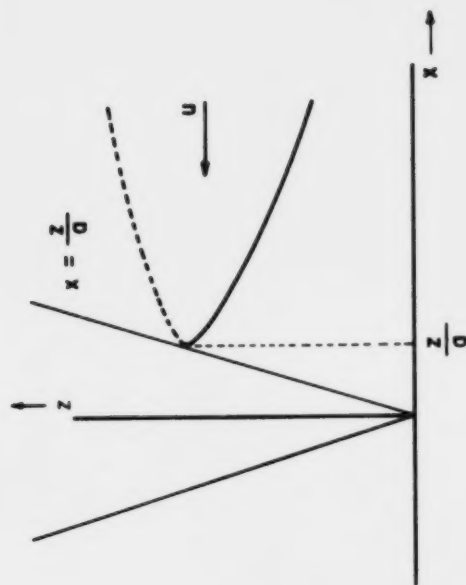


FIGURE 6: DOPPLER SURFACE INTERSECTION
WITH EDGE OF VERTICALLY POINTING
SOUNDER WITH HORIZONTAL WIND.

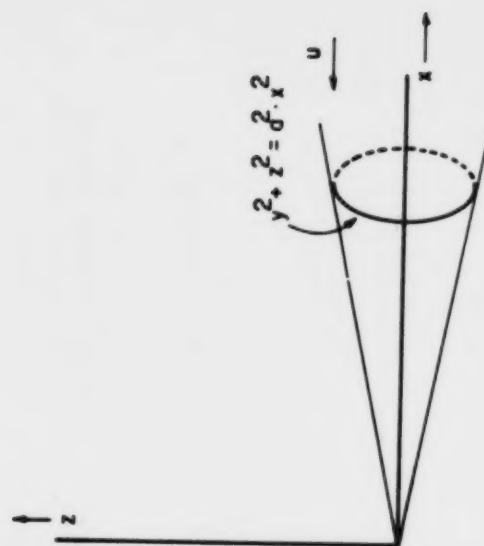


FIGURE 6A : HORIZONTAL WIND AND HORIZONTAL TRANSMITTER-RECEIVER.

Now point the antenna horizontally (or, have a vertical wind only) (Fig. 6A). At any given value of x , the CODOSS is the edge of a circle given by

$$y^2 + z^2 = a^2 x^2$$

Thus, setting the radius equal to the beam edge

$$ax = x \tan \alpha$$

$$\frac{4v^2}{\lambda^2 f^2} = 1 + \tan^2 \alpha$$

$$f = \pm \frac{2v}{\lambda} \cos \alpha$$

where now the plus or minus refers to the beam pointed into the wind or with it, i.e., if we are pointing into the wind, the minimum f is $\frac{2v}{\lambda} \cos \alpha$ while the maximum is given by $ax = 0$,

$$\rightarrow \frac{4v^2}{\lambda^2 f^2} - 1 = 0 \rightarrow f = \pm \frac{2v}{\lambda}$$

When the transmitter is pointed between 0 and 90° with respect to the horizontal wind, analysis is not quite so simple. Assume the transmitter has a boresight at an angle ϕ with respect to the horizontal wind axis (x axis). Now, as in Figure (7), we change our coordinate

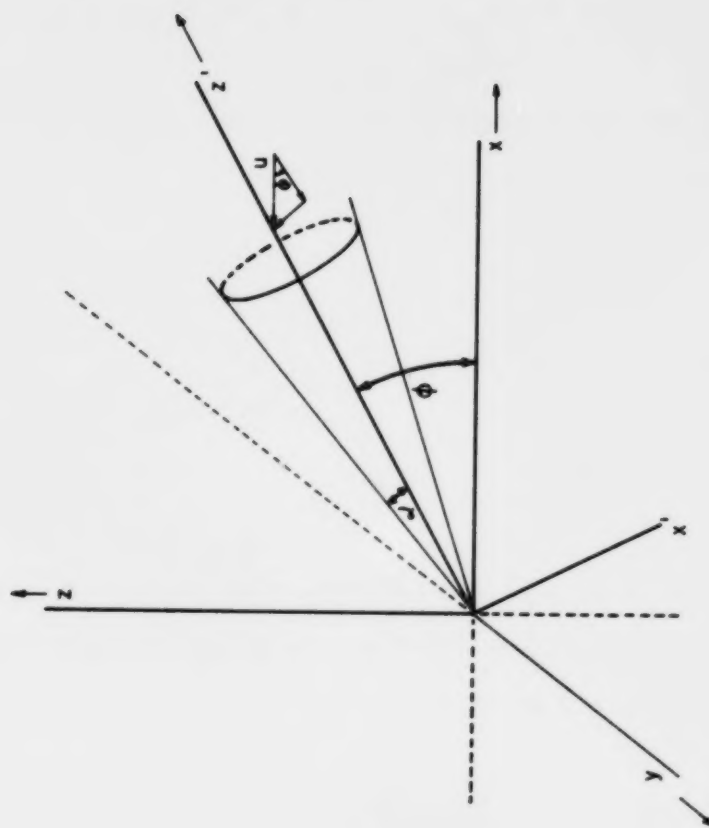


FIGURE 7: PRIMED COORDINATE SYSTEM FOR HORIZONTAL WIND AND SOUNDER BETWEEN THE VERTICAL AND HORIZONTAL AXES.

system such that the x' axis points along the boresight of the transmitter-receiver and the y' axis is perpendicular to the boresight, i.e., we rotate about the y axis by an angle $\phi - \frac{\pi}{2}$.

The horizontal wind (u) can be broken up into components $u_z = u \cos \phi$ and $u_y = u \sin \phi$, and there will be two contributions to the Doppler spectrum, one arising from u_z , (denoted parallel) and another from u_x (denoted perpendicular)

Parallel

The parallel contribution is due to that component parallel to the beam axis and it leads as before to hyperbolas about the z' axis (along the beam) governed by

$$a_{11}^2 z'^2 - y'^2 = x_o'^2$$

where now

$$a_{11}^2 \equiv \frac{4 u_z'^2}{f^2 \lambda^2} - 1 = \frac{4 u^2 \cos^2 \phi}{f^2 \lambda^2} - 1$$

Just as with the horizontally pointing beam, then, the minimum values of f are determined by the value of a_{11} such that the asymptote matches the edge of the beam, i.e.,

$$\frac{x'}{a_{11}} = z' = \frac{x'}{\tan(\alpha)} \quad a = \tan(\alpha)$$

$$f_{\min} = \frac{2u}{\lambda} \cos \phi \cos \alpha$$

$$f_{\max} = \frac{2u}{\lambda} \cos \phi$$

Perpendicular ($a_{\perp}^2 x'^2 - y'^2 = z'^2$)

For this component we have the vertically pointing sounder with horizontal wind. The maximum and minimum frequencies are determined by the intersection point ($y = 0$) of the hyperbola at a given distance

$$z' \tan \alpha = \frac{z'^2}{a_{\perp}^2}$$

$$a_{\perp}^2 = \cot^2 \alpha \rightarrow f_{\pm} = \pm \frac{2u}{\lambda} \sin \phi \sin \alpha$$

$$a_{\perp}^2 = \frac{4u^2}{f^2 \lambda^2} \sin^2 \phi - 1$$

In order to calculate the spectrum, the total area of each CODOSS within the volume bounded by the transmitter beam and the instantaneous scattering length along the beam axis (i.e., inst. scattering length $= \frac{v_p \tau}{2}$, v_p = speed of sound, τ = pulse length (sec.)) must be found.

At a given range (z' in the rotated coordinate system) the parallel component is determined by

$$a_{\parallel}^2 z'^2 - x'^2 = y'^2$$

or

$$x'^2 + y'^2 = a_{\parallel}^2 z'^2$$

which, at any given range z' is a circle; and within the whole volume, is the surface of a truncated rt. circular cone with apex at the coordinate origin (i.e. radius $\rightarrow 0$ as $z' \rightarrow 0$), not including the area of the base.

So the length of the line at distance z' is $S = 2\pi a_{11} z'$ and the surface area is given by

$$A = \int S dl = \int S \frac{dl}{dz'} dz'$$

$$\frac{dl}{dz} = \frac{1}{\cos \gamma} = \frac{1}{z' / (x^2 + z'^2)^{1/2}} = \left(\frac{x^2}{z'^2} + 1 \right)^{1/2} = (a_{11}^2 + 1)^{1/2}$$

$$\rightarrow A = 2\pi \rightarrow \int_{z_1}^{z_2} a_{11} z (a_{11}^2 + 1)^{1/2} dz = \pi a_{11} (a_{11}^2 + 1)^{1/2} (z_2^2 - z_1^2)$$

but

$$z_2 - z_1 = \frac{\ell}{2} = \frac{v \tau}{2}; \quad A = \frac{\pi}{2} \ell a_{11} (a_{11}^2 + 1)^{1/2} (z_2^2 + z_1^2) \\ = \pi \ell a_{11} (a_{11}^2 + 1)^{1/2} z_m^2$$

where z_m is the middle of the volume.

This weighting factor would be the only areal one for the case of a vertically pointing antenna with a vertical velocity alone. Given a Doppler shift, a_{11} is specified and, thus, so is the weighting function in an atmosphere with no horizontal wind and no change of vertical velocity with height. This is, without a doubt, oversimplified, but at least provides a starting point.

In the case of a_1 , things are not so simple. The problem is to determine the length of the hyperbola within a circle of a given radius (Fig. 8), i.e., the hyperbola intersects the circle at points determined by

$$x^2 + y^2 = z^2 \tan^2 \alpha$$

and

$$a_1^2 x^2 - y^2 = z^2$$

combining

$$x^2 = z^2 (1 + \tan^2 \alpha) / (1 + a_1^2)$$

Thus, there are two intersection values of x , corresponding to f_D greater than, or less than, zero. And for each value of x ,

$$y^2 = r^2 - x^2 = z^2 (\tan^2 \alpha - \frac{(1 + \tan^2 \alpha)}{(1 + a_1^2)}) = z^2 \left(\frac{1 + a_1^2 \tan^2 \alpha}{1 + a_1^2} \right)$$

The length of the line is twice the length of the line from $x_1 (y = 0)$ to $x_2 = z^2 (1 + \tan^2 \alpha) / (1 + a_1^2)$. At any point, the infinitesimal length of the line is

$$ds = (1 + (\frac{dy}{dx})^2)^{1/2} dx \text{ where } y^2 = a_1^2 x^2 - z_0^2$$

$$2y dy = 2a_1^2 x dx; \frac{dy}{dx} = a_1^2 \frac{x}{y} = a_1^2 \frac{x}{(a_1^2 x^2 - z_0^2)^{1/2}}$$

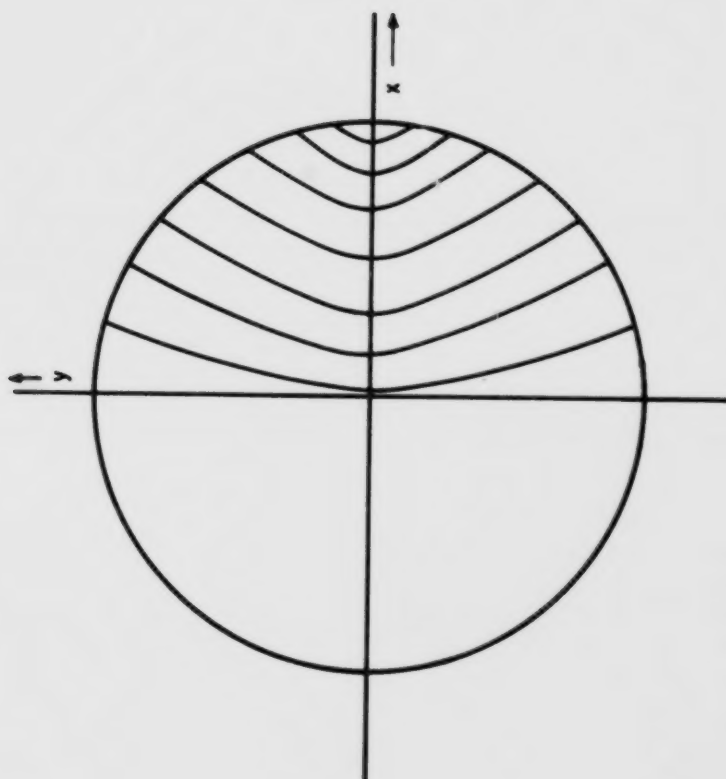


FIGURE 8 : OVER EXAGGERATED VIEW OF HYPERBOLAS DUE TO σ_1 AND CIRCLE SUBTENDED BY TRANSMITTER - RECEIVER CONE. EACH HYPERBOLA REFERS TO A DIFFERENT σ_1 AND THUS A DIFFERENT f_1 .

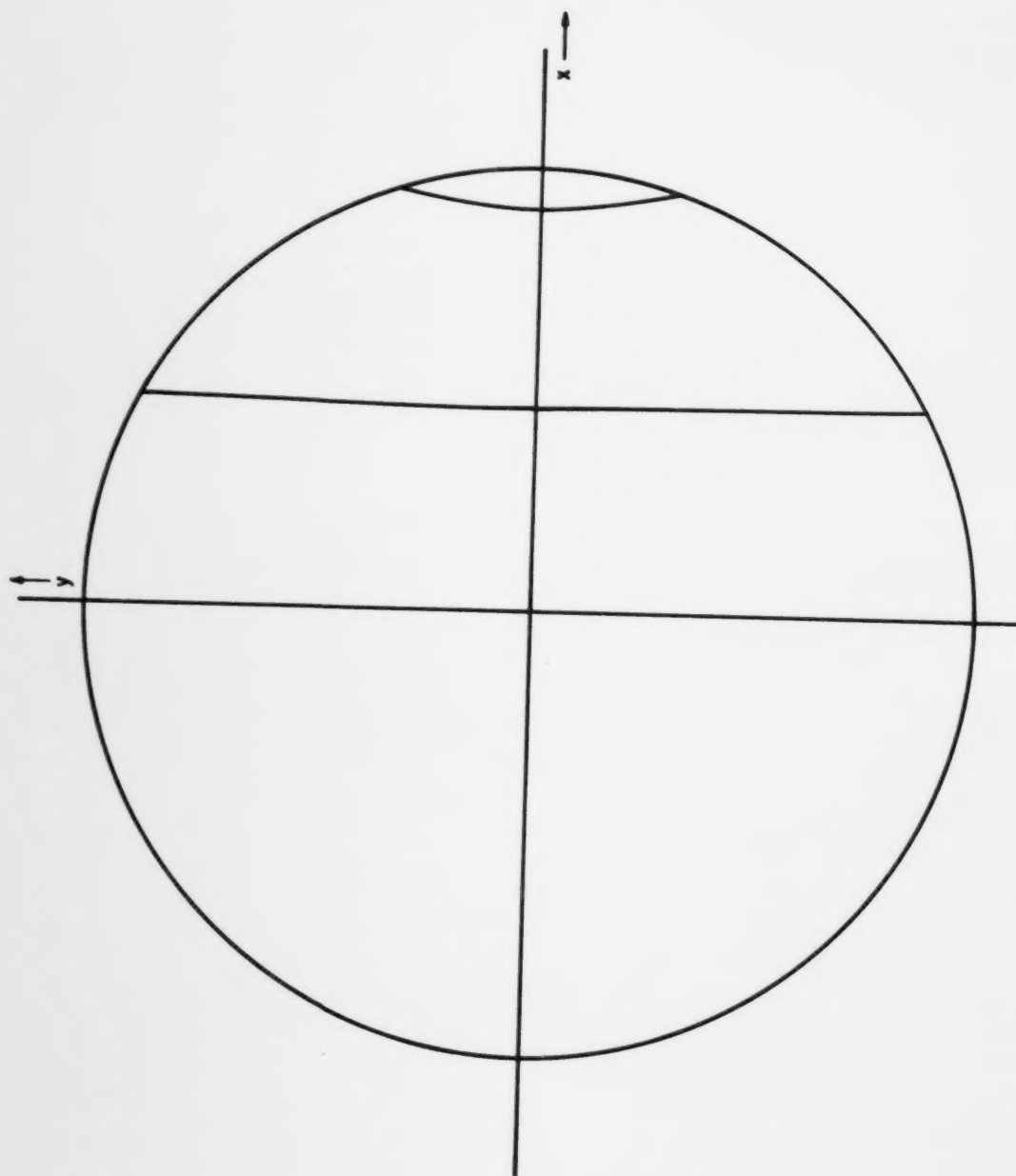


FIGURE 9 : ILLUSTRATING THE ACTUAL RELATION OF THE HYPERBOLA TO CIRCLE USING Q OF 15° . THE DEPARTURE FROM A STRAIGHT LINE IS QUITE SMALL.

$$S = 2 \int_{z_0/a_1}^{x_2} \left(1 + \frac{a_1^4 x^2}{(a_1^2 x^2 - z_0^2)}\right)^{1/2} dx$$

Rather than attempt this integral, it is easier (and perhaps more instructive) to try and approximate the hyperbola by a straight line, noting that the asymptote $x' = \pm \frac{1}{a_1} y$ has a slope

$$\frac{dy}{dx} = \pm a_1$$

which has a minimum value $\cot \alpha$ (i.e., at $x \sim r$). Even if α were as large as 15° , $\cot \alpha \approx 3.7$ which is quite large and thus the hyperbola itself, even though it has slope changing from ∞ to 4, hasn't curved much by the time it reaches the edge of the circle. More precisely, compare the value of x_1 and x_2 :

$$x_1 = z/a_1; \quad x_2 = z \left(\frac{1 + \tan^2 \alpha}{1 + a_1^2} \right)^{1/2}; \quad \text{Def. } \tan^2 \alpha = w$$

$$x_2 \sim \frac{z}{a_1} \left(1 + \frac{1}{2} w - \frac{1}{8} w^2 + \frac{1}{16} w^3 + \dots \right) \cdot$$

$$\left(1 - \frac{1}{2} \frac{1}{a_1^2} + \frac{3}{8} \frac{1}{a_1^4} - \frac{5}{8} \frac{1}{a_1^6} + \dots \right)$$

$$\sim \frac{z}{a} \left(1 - \frac{1}{2a_1^2} + \frac{w}{2} + \frac{3}{8a_1^4} - \frac{w^2}{8} - \frac{w}{4a_1^2} \dots \right) \sim \frac{z}{a_1} \left(1 - \frac{1}{2} \left(\frac{1}{a_1^2} - \tan^2 \alpha \right) \right)$$

$$x_2 - x_1 \sim \frac{z}{2a_1} \left(\frac{1}{a_1^2} - \tan^2 \alpha \right) + \frac{x_2 - x_1}{x} \approx \frac{1}{2} \left(\frac{1}{a_1^2} - \tan^2 \alpha \right)$$

and, percentagewise, $x_2 - x_1$ is quite small.

There are two approximations to straight lines available; one uses the length between x_2 and x_1 ; the other the length of the line perpendicular to the x axis at z_0/a and intersecting the circle at $y = r^2 - z^2/a^2$.

It can be shown that the first approximation yields

$$S_1 = ((x_2 - x_1)^2 + y^2)^{1/2} = \frac{z}{(1 + a_1^2)^{1/2}} \left\{ \frac{1}{4a_1^2} - \left(\frac{1}{a_1^2} - a_1 \tan^2 \alpha \right)^2 + a_1^2 \tan^2 \alpha + 1 \right\}^{1/2}$$

The second, obviously is

$$S_2 = ((x_2 - x_1)^2 + y^2)^{1/2} = y = z \left(\tan^2 \alpha - \frac{1}{a_1^2} \right)^{1/2}$$

Either case is easily integrated

$$A = 2 \int_{z_1}^{z_2} S \frac{dl}{dz} dz = 2S \left(1 + \frac{1}{a_1^2} \right)^{1/2} \left(\frac{z_2^2}{2} - \frac{z_1^2}{2} \right) = S \left(1 + \frac{1}{a_1^2} \right)^{1/2} \ell z_m$$

$$\text{i.e.,} \quad A_1 = \ell z_m \left(1 + \frac{1}{a_1^2} \right)^{1/2} \left(\tan^2 \alpha - \frac{1}{a_1^2} \right)^{1/2}$$

$$A_2 = \ell z_m \left(\frac{1}{4a_1^2} \left(\frac{1}{a_1} - a_1 \tan^2 \alpha \right)^2 + a_1^2 \tan^2 \alpha + 1 \right)^{1/2}$$

Using A_2 we can summarize

$$A_{||} = \pi \ell z_m a_{||} (a_{||}^2 + 1)^{1/2}; \quad 0 \leq a_{||} \leq \tan \alpha$$

$$A_{\perp} = \ell z_m \left(1 + \frac{1}{a_1^2} \right)^{1/2} (\tan^2 \alpha) - \frac{1}{a_1^2}^{1/2}; \quad \cot \alpha \leq a_1 \leq \infty$$

where

$$a_{||}^2 = \frac{4u^2 \cos^2 \phi}{f^2 \lambda^2} - 1; \quad a_{\perp}^2 = \frac{4u^2 \sin^2 \phi}{f^2 \lambda^2} - 1$$

$A_{||}$ is a maximum when $a_{||}$ is a maximum, namely $\tan \alpha$. $A_{\perp}$ is a maximum when $a_{\perp}$ is ∞ . The ratio of the maxima then is

$$\frac{A_{\perp}}{A_{||}} = \frac{\ell z_m \tan \alpha}{\pi \ell z_m \frac{\tan \alpha}{\cos \alpha}} = \frac{\cos \alpha}{\pi}$$

i.e., not including antenna weighting, the contribution at $\phi = 45^\circ$ due to the areal weighting of the parallel component has a peak about 3 times as great as that from the perpendicular. The $\frac{1}{\pi}$ factor is due to the ratio of the circumference of a circle to the diameter and the $\cos \alpha$ is due to the parallel contribution integration at maximum being along the outside surface of the cone while the perpendicular is along the axis (i.e., at an angle of α to the parallel integration).

The frequency range of the two contributions is not, in most cases, coincident. In the perpendicular case, the max and min are given by

$$f_{\perp} = \pm \frac{2u}{\lambda} \sin \phi \sin \alpha$$

while in the parallel case they are

$$f_{\parallel \text{ max}} = \frac{2u}{\lambda} \cos \phi$$

$$f_{\parallel \text{ min}} = \frac{2u}{\lambda} \cos \phi \cos \alpha$$

Thus, for overlap

$$\cos \phi \cos \alpha < \sin \phi \sin \alpha$$

or

$$\tan \phi > \cot \alpha$$

$$\tan \phi > \tan \left(\frac{\pi}{2} - \alpha \right) \rightarrow \phi > \frac{\pi}{2} - \alpha$$

which would require $\phi \sim \frac{\pi}{2}$ if α were small, i.e., almost a vertically pointing antenna.

In an obvious extension, if the transmitter-receiver were pointed off the wind axis, there would be a third component to the spectrum. All previous results hold with the redefinition

$$a_{11}^2 = \frac{u^2 \cos^2 \theta \cos^2 \phi}{f^2 \lambda^2} - 1; \quad a^2 = \frac{u^2 \cos^2 \theta \sin^2 \phi}{f^2 \lambda^2}$$

and now

$$A_{12} = \ell z_m \left(\tan^2 \alpha - \frac{1}{2} \right)^{1/2}; \quad a_{12}^2 = \frac{u^2 \sin^2 \theta}{f^2 \lambda^2} - 1$$

2.4 Antenna Weighting

Any signal received has another variable intrinsic to the system which affects the Doppler spectrum. The power output of the antenna system drops off as one moves away from the boresight (axis of beam). As a general form for this effect, we shall assume it to be Gaussian

$$P = P_o e^{-\alpha'^2 / 2\alpha^2}$$

Thus when $\alpha' = \alpha$ the power incident on that portion of space is about .6 what it was on the beam axis. This term is a function only of the distance from the center. Thus for the parallel contribution, it is easily incorporated. We define the weighting function

$$W_{11}(z, r) = S(z, r) P(z, r)$$

$$= 2\pi (a_{11} z) P_0 e^{-\left(\frac{\alpha'^2}{z^2}\right)}$$

Now α' is determined by the radius of the circle defined by a_{11} , i.e.,

$$\alpha'^2 = \left(\tan^{-1} \frac{r}{z}\right)^2 = \left(\tan^{-1} \left(\frac{x^2 + y^2}{z^2}\right)^{1/2}\right)^2 = \frac{x^2 + y^2}{z^2}$$

but

$$x^2 + y^2 = a_{11}^2 z^2$$

$$W_{11} = 2\pi (a_{11} z) P_0 e^{-\left(\frac{a_{11}^2}{2\alpha^2}\right)}$$

So, integrating in z :

$$W_{11} = 2\pi P_0 \int a_{11} z e^{-\left(\frac{a_{11}^2}{2\alpha^2}\right)} \frac{dz}{dz} dz$$

$$\begin{aligned} W_{11} &= 2\pi P_0 a_{11} (a_{11}^2 + 1)^{1/2} \int_{z_1}^{z_2} z e^{-\left(\frac{a_{11}^2}{2\alpha^2}\right)} \\ &= \pi P_0 a_{11} (a_{11}^2 + 1)^{1/2} 1z_m e^{-\frac{a_{11}^2}{2\alpha^2}} \end{aligned}$$

For the perpendicular contribution, things are not quite so simple, but are straight forward. At a constant z ,

$$\begin{aligned}
 W'(z, \alpha) &= \int S \cdot P dy = 2P_o \int_0^{y(r)} e^{-\frac{\alpha^2}{2\alpha^2} dy} = 2P_o \int e^{-\left(\frac{z^2 + y^2}{2\alpha^2 z^2}\right)} dy \\
 &= 2P_o e^{-\frac{1}{2\alpha^2 a_1^2}} \int e^{-\frac{y^2}{2\alpha^2 z^2}} \text{ bec. } x = \frac{a_1}{z} \text{ in this case.}
 \end{aligned}$$

$$\text{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-u^2} du$$

Define

$$\frac{1}{2\alpha^2} \frac{y^2}{z^2} = u^2 \rightarrow \frac{1}{\alpha^2} \frac{y}{z^2} dy = 2u du; y = \sqrt{2} \alpha z du$$

$$dy = \frac{2u (\alpha^2 z^2) du}{\sqrt{2} \alpha z u} = \sqrt{2} \alpha z du$$

$$\begin{aligned}
 W' &= 2\sqrt{2} P_o e^{-\left(\frac{1}{2\alpha^2 a_1^2}\right)} \alpha z \int_0^v e^{-u^2} du; \\
 v &= \frac{\left(r^2 - \frac{z^2}{a_1^2}\right)^{1/2}}{\sqrt{2} \alpha z} = \frac{\left(\tan^2 \alpha - \frac{1}{a_1^2}\right)^{1/2}}{\alpha \sqrt{2}}
 \end{aligned}$$

$$W' = \sqrt{2\pi} P_o e^{-\frac{1}{2\alpha^2 a_1^2}} \alpha z \text{erf}(v)$$

Integrating in z , then,

$$W_{\perp}(a_{\perp}, \alpha) = \sqrt{\frac{\pi}{2}} P_0 e^{-\left(\frac{1}{2\alpha^2 a_{\perp}^2}\right)\alpha} \operatorname{erf}(v) z_m \ell \left(1 + \frac{1}{2}\right)^{1/2}$$

2.5 Total Spectrum

The complete spectrum due to scatters filling the scattering volume of a monostatic sounder is not just the simple combination of $W_{\parallel}$ and $W_{\perp}$. Any given scatterer will at any instant have a total Doppler shift equal to the sum of $f_{\parallel}$ and $f_{\perp}$. Thus, the contour must be established such that $f_{\parallel} + f_{\perp} = \text{const.}$ and its area calculated.

This is not to say that $f_{\parallel}$ and $f_{\perp}$ are not useful, for they are the limiting cases, and very important ones at that. When $\phi = \frac{\pi}{2}$, there is no Doppler shift due to a parallel component because the wind is horizontal - thus, the only spectrum is that due to $f_{\perp}$ and we have the case of no vertical wind with a vertically pointing monostatic sounder. If $\phi = 0$, the spectrum due to $f_{\perp}$ is zero because the wind is directly along the beam axis. Naturally, no acoustic sounder points horizontally, but the solution to this case ($f_{\parallel}$ only, $\phi = 0$, horizontal wind) is precisely that of a constant vertical wind with a vertically pointing sounder.

Let us consider now the total spectrum with a monostatic sounder pointed off the vertical, but in the plane of the wind vector, whose magnitude and direction is constant with height. At any point, the Doppler shift is

$$f = -\frac{2}{\lambda} \frac{u_z z + u_x x}{(x^2 + y^2 + z^2)^{1/2}}$$

where now z refers to the direction along the beam axis and x is the direction perpendicular to this axis; y is perpendicular to the horizontal wind vector. Rewritten, at a constant z :

$$f = f(r) + g(r) \sin \theta$$

where r refers to the radial distance perpendicular to the beam axis and θ is an angle defined in this plane originating at the y axis as in Fig. (10A). In other words, f is the shift due to the parallel component and f_2 is that due to the perpendicular component. We can write f as

$$f_1 = \frac{-2u \cos \phi}{\lambda} \cos \alpha'$$

where α' is an angle taking on values between α and $-\alpha$ (Fig. 10B) and

$$f_2 = - \frac{2u \sin \phi}{\lambda} \sin \alpha'$$

The total change in f_1 across the plane is, in most cases, much less than the change in f_2 because $\cos \alpha'$ changes from $\cos(0)$ to $\cos(\alpha)$ while $\sin \alpha'$ changes from $-\sin(\alpha)$ to $+\sin \alpha$ and $\sin \alpha$ changes much more rapidly as α' varies about 0. The only point where this doesn't apply is when ϕ approaches $\pi/2$, and $\cos \phi \rightarrow 0$ and the f_2' variation becomes small. With this in mind, then, we will try as a curve of constant Doppler shift a

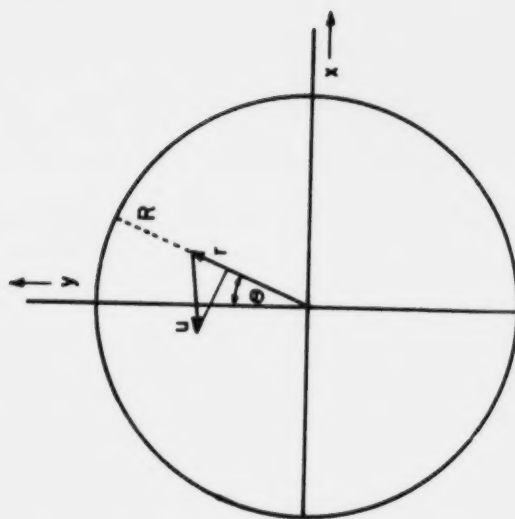


FIGURE 10A : HEAD ON VIEW OF CIRCLE
SUBTENDED BY TRANSMITTER CONE
AND ILLUSTRATING COMPONENT OF u
ALONG r .

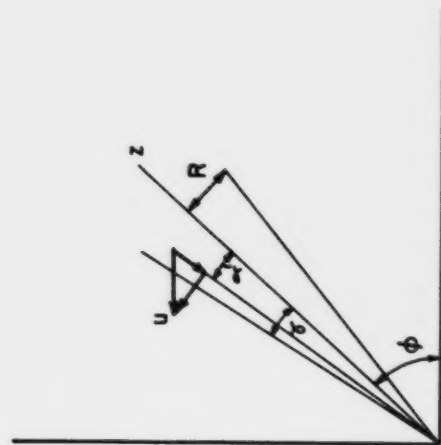


FIGURE 10B : SIDE VIEW OF BEAM SHOWING
RELATION OF α' TO α . α' IS MEASURED
AS POSITIVE IN THE CLOCKWISE FROM
THE z AXIS.

straight line (Fig. 11). In order to determine the slope we set the total Doppler frequency at $y = 0$ equal to that at $y(r)$ where r is the radius of the beam at any given z . At this point we shall use, rather than a circle of radius $z \tan \alpha$, one of radius $z \tan(3\alpha)$. The reason for this will become apparent later, but suffice it to say that in the final result, one may replace 3α with α and the results will be equally correct so far as calculating the equation of the straight lines is concerned.

Thus

$$\begin{aligned} f\left(\begin{matrix} \theta = \pi/2 \\ y = 0 \end{matrix}\right) &= f(r) \\ &= -\frac{2u}{\lambda} (\cos \phi \cos \alpha' + \sin \phi \sin \alpha') \\ &= -\frac{2u}{\lambda} (\cos \phi \cos 3\alpha + \sin \phi \sin 3\alpha \sin \theta) \end{aligned}$$

The left side is

$$\begin{aligned} &= -\frac{2u}{\lambda} \left(\cos \phi \frac{z}{(x^2 + z^2)^{1/2}} + \sin \phi \frac{x}{(x^2 + z^2)^{1/2}} \right) \\ &= -\frac{2u}{\lambda} \left(\cos \phi \frac{1}{\left(\frac{x^2}{z^2} + 1\right)^{1/2}} + \sin \phi \frac{x/z}{\left(\frac{x^2}{z^2} + 1\right)^{1/2}} \right) \end{aligned}$$

That is, given $y = 0$, the x intercept can be written in terms of α . Noting that

$$\sin \theta = \frac{x}{r} = \frac{x}{z \tan 3\alpha}$$

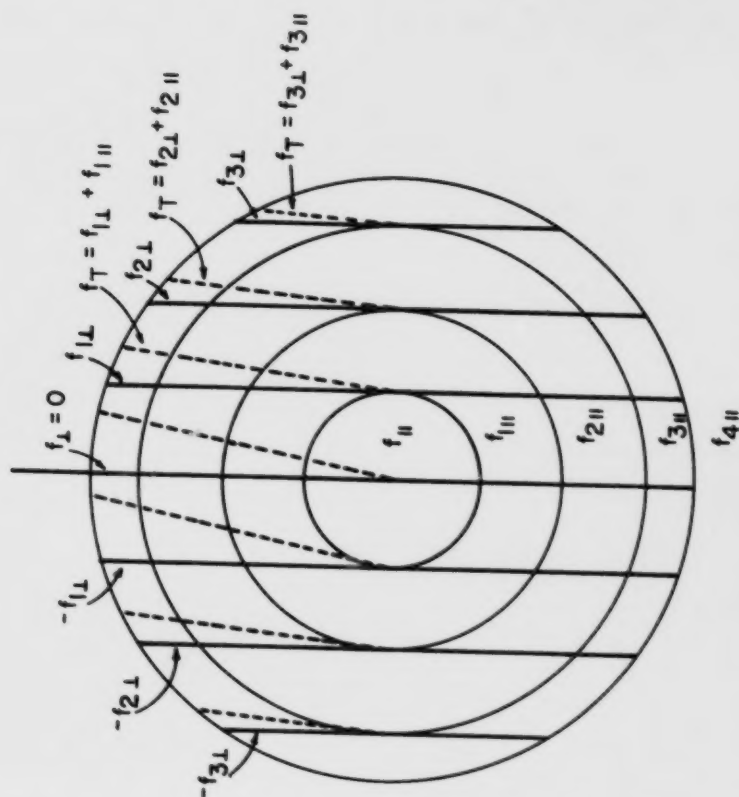


FIGURE II : DEPICTION OF LINES OF CONSTANT TOTAL SHIFT AS WELL AS f_L LINES AND f_H .

$$\frac{a_{\perp}}{(1 + a_{\perp}^2)^{1/2}} \cos \phi + \frac{1}{(1 + a_{\perp}^2)^{1/2}} \sin \phi = \cos \phi \cos 3\alpha$$

$$+ \sin \phi \sin (3\alpha) \frac{x}{z \tan (3\alpha)}$$

$$\frac{1}{(1 + a_{\perp}^2)^{1/2}} (a_{\perp} \cos \phi + \sin \phi) - \cos \phi \cos (3\alpha) = \frac{x}{z} \sin \phi \cos (3\alpha)$$

Thus

$$x(r, a_{\perp}) = z \left\{ \frac{a_{\perp} \cot \phi + 1}{(1 + a_{\perp}^2)^{1/2} \cos (3\alpha)} - \cot \phi \right\}$$

The slope of the line is then

$$\frac{\Delta x}{\Delta y} \equiv a = \frac{\left(\frac{a_{\perp} \cot \phi + 1}{(a_{\perp}^2 + 1)^{1/2} \cos (3\alpha)} - \cot \phi \right) - \frac{1}{a_{\perp}}}{\left[\tan^2 (3\alpha) - \left\{ \frac{a_{\perp} \cot \phi + 1}{(a_{\perp}^2 + 1) \cos (3\alpha)} - \cot \phi \right\}^2 \right]^{1/2}}$$

and we can easily find its length. One should note, however, that the Doppler frequency to which this line corresponds is not that associated with $a_{\perp}$, but rather the f calculated from

$$f = \frac{2u}{\lambda} (\sin \phi \sin \alpha' + \cos \phi \cos \alpha')$$

where α' is determined by $a_{\perp}$.

Rather than calculate step by step the area for a given CODOSS without the antenna weighting included, the result is just given

$$A = \frac{\ell z}{2} \left\{ \tan^2 (3\alpha) + \frac{1}{a_{\perp}^2} + \frac{2\eta}{a_{\perp}} \right\}^{1/2} \left(1 + \frac{1}{a_{\perp}^2} \right)^{1/2}$$

where

$$\eta = \sec (3\alpha) \frac{\cot \phi + 1/a}{(1 + 1/a_{\perp}^2)^{1/2}} - \cot \phi = \frac{x(r)}{z}$$

2.6 With Antenna Weighting

$$ds = 2 dy \left(1 + \left(\frac{dx}{dy} \right)^2 \right)^{1/2}$$

$$= 2 dy (1 + a^2)^{1/2}$$

So

$$W' = P_o \int e^{-\left(\frac{\alpha^2}{2\alpha^2}\right)} ds = 2 P_o \int_0^{y(r)} \exp\left(-\frac{1}{2\alpha^2} \left(\frac{x^2 + y^2}{z^2}\right)\right) (1 + a^2) dy$$

Now the line of constant Doppler shift is defined by

$$= \frac{z}{a_{\perp}} + ay \rightarrow x^2 = \left(\frac{z}{a_{\perp}} + ay \right)^2$$

Then

$$W' = 2P_o \int \exp \left(- \frac{1}{2\alpha^2 z^2} \left\{ \left(\frac{z}{a_1} + ay \right)^2 + y^2 \right\} \right) (1 + a^2)^{1/2} dy$$

By completing the square, we may rewrite the exponential term as

$$\exp \left[- \frac{1}{2\alpha^2} \left\{ ([1 + a^2]^{1/2} \frac{y}{z} + \frac{1}{a_1} \frac{a}{(1 + a^2)^{1/2}})^2 + \frac{1}{a_1^2} \frac{1}{(1 + a^2)} \right\} \right]$$

Defining

$$\gamma = \frac{(1 + a^2)^{1/2}}{z} ; \quad \delta = \frac{a}{a_1 (1 + a^2)^{1/2}} ; \quad \beta^2 = \frac{1}{a_1^2 (1 + a^2)}$$

we can write

$$W' = 2P_o (1 + a^2)^{1/2} e^{-\left(\frac{\beta^2}{2\alpha^2}\right)} \int_{y_1}^{y_2} \exp \left(- \frac{1}{2\alpha^2} (\gamma y + \delta)^2 \right) dy$$

Then

$$\frac{\gamma y + \delta}{\sqrt{2}\alpha} \equiv u, \quad \frac{\gamma dy}{\sqrt{2}\alpha} = du \rightarrow dy = \frac{\alpha\sqrt{2}}{\gamma} du$$

and

$$W' = 2\sqrt{2} P_o \alpha \frac{(1 + a^2)^{1/2}}{\gamma} e^{-\frac{\beta^2}{2\alpha^2}} \int_{u_1}^{u_2} e^{-u^2} du$$

where

$$u_1 = \frac{\delta}{\alpha\sqrt{2}} = \frac{a}{a_1 (a^2 + 1)^{1/2} \alpha\sqrt{2}}$$

$$u_2 = \frac{\gamma y_2 + \delta}{\alpha\sqrt{2}} = (1 + a^2)^{1/2} \eta - \frac{a^2}{a_1 (1 + a^2)^{1/2}} ;$$

$$y_2 = z (\tan^2 (3\alpha) - \eta^2)^{1/2}$$

Thus, noting the definition of γ ,

$$W' = \sqrt{2\pi} \alpha e^{-\frac{\beta^2}{2\alpha^2} z} \{ \operatorname{erf}(u_2) - \operatorname{erf}(u_1) \}$$

Integrating in z we get

$$W = \sqrt{\frac{\pi}{2}} \alpha e^{-\left(\frac{\beta^2}{2\alpha^2}\right) z} \{ \operatorname{erf}(u_2) - \operatorname{erf}(u_1) \} \ell z_m \alpha$$

Spectra for varying ϕ_1 , α_1 are depicted in Figures ((12) - (15)) as calculated from the previous equations. It is in the calculation of these spectra that the necessity to include scatters out to 3α rather than just to α in order to include enough of the wings of the spectra arises. Of course, in addition to the antenna weighting, contributions from the side lobes should be considered. The easiest method for calculating lobe effects is to use step functions; i.e., assume each lobe has constant power up to a certain angle (α), and then cuts to zero for the same angle, etc. etc.. If one does this and recalculates the spectrum, the result is

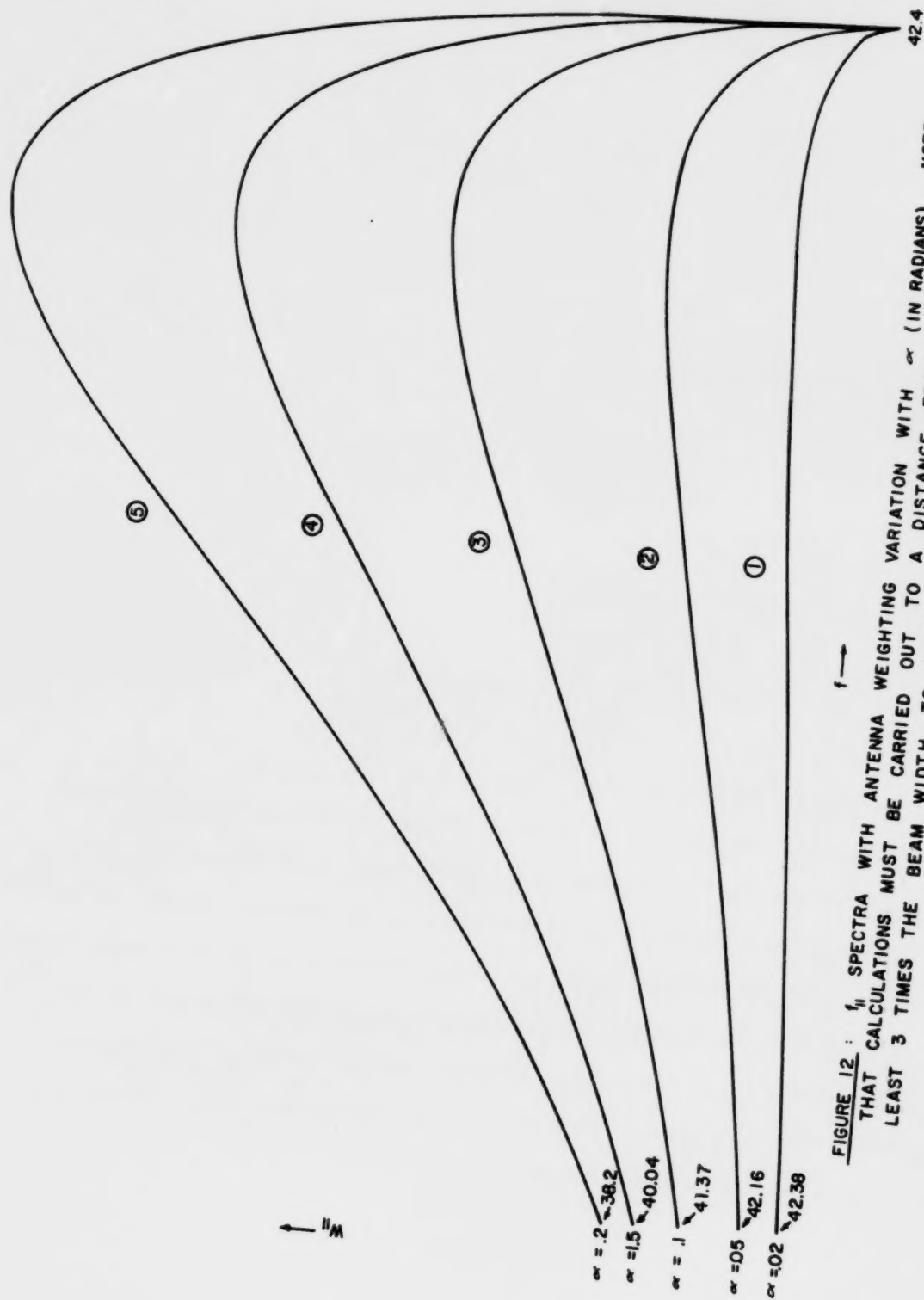


FIGURE 12 : f_{11} SPECTRA WITH ANTENNA WEIGHTING VARIATION WITH α (IN RADIAN). NOTE THAT CALCULATIONS MUST BE CARRIED OUT TO A DISTANCE FROM BORE SIGHT AT LEAST 3 TIMES THE BEAM WIDTH TO INCLUDE THE FULL SPECTRUM. $z, l, u, \phi, \lambda = \text{CONSTANT}$.



FIGURE 13 : f_{II} SPECTRUM VARYING ϕ . NOTE THAT, ALTHOUGH SPECTRA OVERLAP, THE ABCISSA CHANGES IN EACH CASE. FOR $\phi = 0$, $f_{min} = 58.5$, $f_{max} = 60$. FOR $\phi = 10$, $f_{min} = 57.6$, $f_{max} = 59.1$. FOR $\phi = 26$, $f_{min} = 51.05$, $f_{max} = 52.4$. ALSO NOTE THAT THE $\phi = 0$ CURVE REPRESENTS THAT WHICH WOULD BE OBTAINED FROM A VERTICALLY POINTING SOUNDER WITH VERTICAL WIND. $\alpha_z, l, u, \phi, \lambda = \text{CONSTANT}$.



FIGURE 14: f_1 SPECTRUM FOR $\phi = \frac{\pi}{2}$ AND HORIZONTAL WIND OF 10 m/sec.

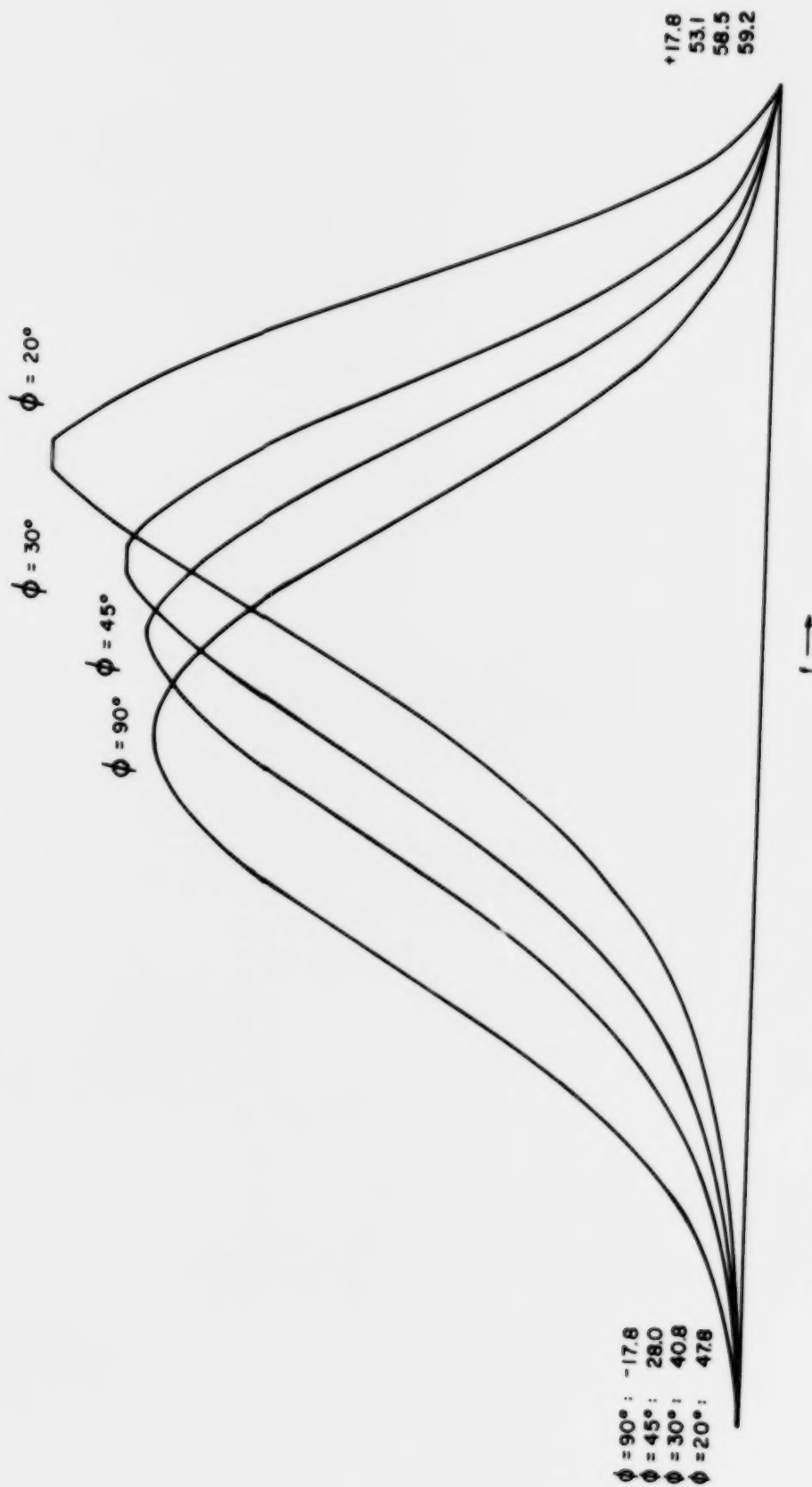


FIGURE 15 : TOTAL SPECTRA AND VARIATION WITH ϕ . NOTE INCREASE IN HEIGHT OCCURS AS ϕ APPROACHES 20° DUE TO INACCURACIES IN APPROXIMATION. ALSO NOTE THE CHANGE IN SHAPE AS f_L DOMINATES ($\phi \sim 90^\circ$) AND f_H INCREASES IN CONTRIBUTION ($\phi \rightarrow 0$).



FIGURE 16 : TOTAL f INCLUDING ANTENNA WEIGHTING AND LOBE WEIGHTING
FOR $\theta = 45^\circ$, $\alpha = 5^\circ$.

$$W(z, \alpha) = \sqrt{\frac{\pi}{2}} P_0 e^{-\frac{\beta^2}{2\alpha^2}} \lambda z_m \alpha \{ \operatorname{erf}(\mu_1) + \operatorname{erf}(\mu_2) - \operatorname{erf}(\mu_2) - \operatorname{erf}(\mu_1) \}$$

where

$$\mu_1^2 = \frac{\tan^2 \alpha' - \beta^2}{2\alpha^2} ; \mu_2^2 = \frac{\tan^2 (2\alpha') - \beta^2}{2\alpha^2}$$

$$\mu_3^2 = \frac{\tan^2 (3\alpha') - \beta^2}{2\alpha^2}$$

An example of this is shown in Fig. (16). Now, we see the possibility of more than one peak appearing in the spectrum. The reason, of course, is the cutting out of part of the input spectrum between α and 2α .

2.7 Wind Shear Included

The inclusion of wind varying with height is not a trivial problem, Analytically, things rapidly get out of hand and some simplifying assumptions are required. Although an alternate approach is, of course, to use a computer, this does not yield a comparable understanding of the physics of the problem.

Parallel Component

We go back to the equation

$$a_{11}^2 z^2 = x^2 + y^2$$

where

$$a_{11}^2 = \frac{4u^2 \cos^2 \phi}{f_{11}^2 \lambda^2} - 1$$

only now u is a function of z , and therein lies the problem. Let

$$u = kh; \quad h = \text{height above ground}$$

and

$$c_{11}^2 = \frac{4k^2 \cos^2 \phi}{f^2 \lambda^2}$$

$$(c_{11}^2 h^2 - 1) z^2 = x^2 + y^2$$

Now

$$h = z \sin \phi - x \cos \phi$$

Then

$$\{c_{11}^2 (z^2 \sin^2 \phi + x^2 \cos^2 \phi - 2xz \sin \phi \cos \phi) - 1\} z^2 = x^2 + y^2$$

and things have rapidly become much more complicated. Note, however, that the maximum absolute value for x is $z \tan \alpha$ which becomes for narrow beams ($\alpha < 5^\circ$) $x \leq .1z$. So, in order to simplify things write

$$h \approx z \sin \phi$$

$$(c_{11}^2 z^2 \sin^2 \phi - 1) z^2 = x^2 + y^2$$

This, again is the form for a circle of radius

$$z(c_{11}^2 z^2 \sin^2 \phi - 1)^{1/2}$$

and we can write, for the length of the CODOSS at a given z :

$$S = 2\pi z (c_{II}^2 z^2 \sin^2 \phi - 1)^{1/2}$$

Now, if we use, as before,

$$\frac{dl}{dz} = \frac{1}{\cos \gamma} = \frac{1}{z/(x^2 + y^2)^{1/2}} = \left(\left(\frac{x}{z}\right)^2 + 1\right)^{1/2}_{y=0}$$

$$= (c^2 z^2 \sin^2 \phi - 1 + 1)^{1/2} = c_{II} \sin \phi$$

This form for $\frac{dl}{dz}$ is not exactly correct. In full form, it turns out to be

$$\frac{dl}{dz} = \{c_{II}^2 z^2 \sin^2 \phi + \frac{c_{II}^4 z^2 \sin^4 \phi}{c_{II}^2 z^2 \sin^2 \phi - 1} + 2c_{II}^2 z \sin^2 \phi\}^{1/2}$$

We have, thus far, kept only the first term. This has had consequences mainly for those CODOSS which are near the axis of the transmitter.

Continuing:

$$A = 2\pi c_{II} \sin \phi \int_{z_1}^{z_2} z^2 (c_{II}^2 z^2 \sin^2 \phi - 1)^{1/2} dz$$

$$\begin{aligned}
&= \frac{\pi c_{11}^2 \sin^2 \phi}{2} \left\{ z_2 \left(z_2^2 - \frac{1}{c_{11}^2 \sin^2 \phi} \right)^{1/2} \left(z_2^2 - \frac{1}{2c_{11}^2 \sin^2 \phi} \right) \right. \\
&\quad - z_1 \left(z_1^2 - \frac{1}{c_{11}^2 \sin^2 \phi} \right) \left(z_1^2 - \frac{1}{2c_{11}^2 \sin^2 \phi} \right) \\
&\quad \left. - \frac{1}{2c_{11}^4 \sin^4 \phi} \ln \left(\frac{z_2 + \left(z_2^2 - \frac{1}{c_{11}^2 \sin^2 \phi} \right)^{1/2}}{z_1 + \left(z_1^2 - \frac{1}{c_{11}^2 \sin^2 \phi} \right)^{1/2}} \right) \right\}
\end{aligned}$$

Including Guassian antenna weighting →

$$\begin{aligned}
A &= 2\pi c_{11} \sin \phi \int_{z_1}^{z_2} \exp \left[-\frac{1}{2\alpha^2} (c_{11}^2 z^2 \sin^2 \phi - 1) \right] \\
&\quad z^2 (c_{11}^2 z^2 \sin^2 \phi - 1)^{1/2} dz \\
&= \frac{2\pi}{c_{11}^2 \sin^2 \phi} \int_{x_1}^{x_2} e^{-\frac{x^2}{2\alpha^2}} x^2 (x^2 + 1)^{1/2} dx \text{ where } x^2 = c_{11}^2 z^2 \sin^2 \phi - 1 \\
&\quad 0 \leq x^2 \leq \alpha^2
\end{aligned}$$

If one assumes $0 < x^2 < .01$ ($\alpha < 5^\circ$) this integral can be approximated and done to yield

$$A = \frac{\sqrt{2}\pi^3 \alpha^2 (1 + \alpha^2)}{c_u^2 \sin^2 \phi} \left\{ \alpha \left(\operatorname{erf} \left(\frac{x_2}{\alpha} \right) - \operatorname{erf} \left(\frac{x_1}{\alpha} \right) \right) \right. \\ \left. + x_1 \left(1 + \frac{x_1^2 e^{-\left(\frac{x_1^2}{2\alpha^2}\right)}}{a(1 + \alpha^2)} \right) - x_2 \left(1 + \frac{x_2^2 e^{-\left(\frac{x_2^2}{2\alpha^2}\right)}}{2(1 + \alpha^2)} \right) \right\}$$

Perpendicular Component With Wind Shear

Again, we have

$$a_{\perp}^2 x^2 = z^2 + y^2$$

$$a_{\perp}^2 = \frac{4u^2 \sin^2 \phi}{f^2 \lambda^2} - 1 \quad \vec{u} = \vec{f}(z) \quad b^2 h^2 - \text{where}$$

$$b^2 = \frac{4k^2 \sin^2 \phi}{f^2 \lambda^2}$$

Once again,

$$h = z \sin \phi - x \cos \phi \sim z \sin \phi$$

$$(b^2 z^2 \sin^2 \phi - 1) x^2 = z^2 + y^2$$

or

$$x^2 \left(\frac{b^2 z^2 \sin^2 \phi - 1}{z^2} \right) - \frac{y^2}{z^2} = 1$$

which is another hyperbola at constant z with asymptote

$$x = \pm (b^2 z^2 \sin^2 \phi - 1)^{1/2} y$$

and x intercept ($y=0$)

$$x = \frac{z}{(b^2 z^2 \sin^2 \phi - 1)^{1/2}}$$

For a circle of radius $r = z \tan \alpha$, we get a value of $x = z \tan \alpha$ when $y = 0$, where

$$\tan \alpha = \frac{1}{(b^2 z^2 \sin^2 \phi - 1)^{1/2}}$$

If, as before, the hyperbola length is approximated by a straight line perpendicular to the x axis at x_1 :

$$\frac{1}{2} S_1^2 = r^2 \frac{z^2}{(b^2 z^2 \sin^2 \phi - 1)} = z^2 \left\{ \tan^2 \alpha - \frac{1}{b^2 z^2 \sin^2 \phi - 1} \right\}$$

Then

$$A = \int S_1 dz = 2 \int z \left(\tan^2 \alpha - \frac{1}{b^2 z^2 \sin^2 \phi - 1} \right)^{1/2} dz$$

$$+ \frac{1}{d^2} \left\{ - \frac{(a^2 - u^2)^{1/2}}{u} - \frac{1}{2a} \ln \left(\frac{[a^2 - u]^{1/2} - a}{[a^2 - u]^{1/2} + a} \right) \right\} \quad u_2 = \frac{1}{d^2 z^2 - 1}$$

$$u_1 = \frac{1}{d^2 z^2 - 1}$$

$$\begin{aligned} d^2 &= b^2 \sin^2 \phi \\ \text{with } a^2 &= \tan^2 \phi \end{aligned}$$

Including Gaussian antenna weighting leads to some difficulties,
but an answer can be obtained:

$$S = 2P_o \int_0^{r^2 - \frac{z^2}{(d^2 z^2 - 1)_2}} \exp \left(- \frac{1}{2\alpha^2} \left\{ \frac{x^2 + y^2}{z^2} \right\} \right) = 4P_o \exp \left(- \frac{1}{2\alpha^2 (d^2 z^2 - 1)} \right) \alpha z \cdot$$

$$\int_0^{u_1} e^{-u^2} du$$

where

$$u_1 = \frac{1}{\sqrt{2}\alpha} \left(\tan^2 \alpha - \frac{1}{d^2 z^2 - 1} \right)^{1/2}$$

Then

$$A_1 = 2\sqrt{\pi} P_o \alpha \int_{z_1}^{z_2} z \exp \left\{ - \frac{1}{2\alpha^2} \left(\frac{1}{d^2 z^2 - 1} \right) \right\} \operatorname{erf} (u_1(z))$$

Expanding $\text{erf}(u_1)$ in a McLaurins series and integrating (App. II):

$$A \approx \frac{\sqrt{2} P_0}{d^2} \left\{ \tilde{\alpha} \frac{e^{-\left(\frac{u}{2\alpha}\right)^2}}{u} + \left(\frac{\tilde{\alpha}}{2\alpha^2} - \alpha_1 \right) \left(\ln u - \frac{1}{2\alpha^2} u + \frac{1}{2} \left(\frac{1}{2\alpha} \right)^2 u^2 \right. \right. \\ \left. \left. - \frac{1}{(2.3)} \left(\frac{1}{2\alpha} \right)^3 u^3 + \dots \right) \right\}$$

$$u_2 = \frac{1}{d^2 z^2 - 1}$$

$$u_1 = \frac{1}{d^2 z^2 - 1}$$

The applicability of the last two derivations as they stand is rather limited. This last one is strictly valid only for a vertically pointing sounder. At any other angle the sum of A_{11} and A_{12} must be considered once again. A_{11} is really not valid anywhere, because the only time we have A_{11} only is when $\phi = 0$. At this point the approximation $h = z \sin \phi + x \cos \phi \approx z \sin \phi$ prohibits any variation across the beam of the wind. This case in no wind shear conditions was equivalent to the vertical wind, vertical pointing case, but is no longer. Thus A_{11} cannot be used by itself for any computations. A separate study of this case for w varying with height could and should be done.

Combined Spectrum

In order to try and come to some expression for the total Doppler frequency spectrum, we must go back to essentially the same point from which we started the no shear case.

$$f_T = f(r) + g(r) \sin \theta$$

Constant $f_{||}$ circles at a constant z are defined by

$$r^2 = (c^2 (z - z_0)^2 \sin^2 \phi - 1) z^2; \quad c^2 = \frac{4k^2 \cos^2 \phi}{f_{||}^2 \lambda^2}, \quad u = k(h - h_0)$$

$$h \sim z \sin \phi$$

Constant $f_{\perp}$ lines are determined by straight lines perpendicular to the x axis at

$$\frac{z}{(b^2 (z - z_0)^2 \sin^2 \phi - 1)^{1/2}} \equiv \frac{z}{b}$$

$$s_{\perp} = z \left(\tan^2 \alpha - \frac{1}{b^2 (z - z_0)^2 \sin^2 \phi - 1} \right)^{1/2}$$

Note that now instead of $u = kh$, we have $u = k(h - h_0)$ which does not change the calculations at all.

Taking the same approach we have,

$$f(y = 0) = f(r)$$

$$f(y = 0) = \frac{2u}{\lambda} (\cos \phi \cos \alpha' + \sin \phi \sin \alpha')$$

$$= \frac{2u}{\lambda} \left(\frac{z \cos \phi}{(x^2 + z^2)^{1/2}} + \frac{x \sin \phi}{(x^2 + z^2)^{1/2}} \right)$$

$$= \frac{2u}{\lambda} \left(\frac{\cos \phi}{\left(1 + \frac{1}{b_d^2}\right)^{1/2}} + \frac{\sin \phi}{b_d \left(1 + \frac{1}{b_d^2}\right)^{1/2}} \right)$$

Whence

$$\underbrace{\cos \phi \cos (3\alpha) + \sin \phi \sin (3\alpha)}_{\frac{x}{z \tan(3\alpha)}} \sin \theta(r) = \frac{1}{\left(1 + \frac{1}{b_d^2}\right)^{1/2}} \left(\cos \phi + \frac{1}{b_d} \sin \phi \right)$$

We have, here, made the implicit assumption that $h = z \sin \phi$ because we have cancelled out the u on both sides of the equation while they are not necessarily equal because u changes across the face of the beam.

This leads to

$$\frac{x(r)}{z} = -\cot \phi + \frac{1}{\cos (3\alpha)} \left\{ \cot \phi + \frac{1}{b} \right\} \frac{1}{\left(1 + \frac{1}{b^2}\right)^{1/2}}$$

$$y^2 = r^2 - x^2 = z^2 \left[\tan^2 (3\alpha) - \frac{1}{\cos (3\alpha)} \left(\cot \phi + \frac{1}{b} \right) \left(\frac{1}{\left(1 + \frac{1}{b^2}\right)^{1/2}} - \cot \phi \right)^2 \right]$$

from which we get the slope

$$b = \frac{\Delta x}{\Delta y} = \frac{\frac{(\frac{1}{b} + \operatorname{ctn} \phi)}{\operatorname{Sec}(3\alpha)(1 + 1/b^2)^{1/2} - \operatorname{ctn} \phi - \frac{1}{b}}}{\{\operatorname{Tan}^3(3\alpha) - [\operatorname{Sec}(3\alpha)(\operatorname{ctn} \phi + \frac{1}{b}) \frac{1}{(1 + \frac{1}{b^2})^{1/2} - \operatorname{ctn} \phi}]^2\}^{1/2}}$$

$$\equiv \frac{\beta - \frac{1}{b}}{(\operatorname{Tan}^2(3\alpha) - \beta^2)^{1/2}}$$

This is exactly the same form as previously used. However, now β and b are functions of z . Since they are functions of z and not x or y , we can follow exactly as in the no shear case to the result at constant z :

$$W'(z, \alpha, \phi) = 2P_0 (1 + b^2)^{1/2} e^{-\frac{\beta_1^2}{2\alpha^2}} \int_{y_1}^{y_2} e^{-\frac{1}{2\alpha^2} (\gamma_1 y + \delta_1)^2} dy$$

$$= \sqrt{\frac{\pi}{2}} P_0 e^{-\frac{\beta_1^2}{2\alpha^2}} \alpha \{\operatorname{erf}(\tilde{u}_2) - \operatorname{erf}(\tilde{u}_1)\} z$$

with

$$\beta_1^2 = \frac{1}{b^2 (1 + b^2)} ; \quad \gamma = \frac{(1 + b^2)^{1/2}}{z}$$

$$\delta = \frac{b}{b (1 + b^2)^{1/2}} ; \quad u_1 = \frac{b}{b (1 + b^2)^{1/2} \sqrt{2} \alpha} ;$$

$$u_2 = (1 + b^2)^{1/2} (\operatorname{Tan}^2(3\alpha) - \beta^2)$$

where $\beta = \eta$ with a_1 replaced by b_1 .

Inasmuch as β_1 , u_2 , and u_1 are rather complicated functions of z , the integration in the z direction was carried out numerically. Before this is done, a calculation similar to that for determining the straight line at constant z must be carried out.

At each level along z , the point at which the Doppler frequency remains the same, will determine a new α' (See Fig. 17), which in turn determines a new b_1 and thus, the length of the line at the new level along z . This value is then used in the calculation for the next level and so forth. Specifically, we set the Doppler frequency at level 1 equal to that at level 2 at the point $\theta = \pi/2$, $y = 0$.

$$\frac{2u(z_2)}{\lambda} \{\cos \alpha_2' \cos \phi + \sin \alpha_2' \sin \phi\} = \frac{2u(z_1)}{\lambda} \{\cos \alpha_1' \cos \phi + \sin \alpha_2' \sin \phi\}$$

or

$$\cos(\alpha_2') \cos \phi + (1 - \cos^2(\alpha_2'))^{1/2} \sin \phi = \frac{\lambda}{2u(z_2)} \frac{2u(z_1)}{\lambda}$$

$$\cos(\alpha_1' + \phi) = \frac{\lambda f}{2u(z_2)} \equiv \epsilon$$

because f is the same on both sides.

Then

$$\cos(\alpha_2') \cot \phi - \frac{\epsilon}{\sin \phi} = - (1 - \cos^2 \alpha_2')^{1/2}$$

$$\cos^2(\alpha_2') (1 + \cot^2 \phi) - \cos(\alpha_2') \left(\frac{2\epsilon \cos \phi}{\sin^2 \phi} \right) + \frac{\epsilon^2}{\sin^2 \phi} - 1 = 0$$

Simplifying

$$\cos^2(\alpha_2') - (2\epsilon \cos \phi) \cos(\alpha_2') + \epsilon^2 - \sin^2 \phi = 0$$

Solving

$$\cos(\alpha_2') = \epsilon \cos \phi \pm \sin \phi (1 - \epsilon^2)^{1/2}$$

i.e.,

$$\cos(\alpha_2') = \frac{\lambda f \cos \phi}{2k(z_2 - z_0) \sin \phi} \pm \sin \phi \left(1 - \left(\frac{\lambda f}{2k(z_2 - z_0) \sin \phi} \right)^2 \right)^{1/2}$$

Using this, then, a new α' is calculated at each new level of z . Now

$$b_{\perp} = \left(\frac{4k^2 \sin \phi}{f_{\perp}^2 \lambda^2} (z - z_0)^2 \sin^2 \phi - 1 \right)^{1/2}$$

But

$$f_{\perp} = \frac{2u}{\lambda} \sin \phi \sin \alpha' \rightarrow b_{\perp} = \left(\frac{1}{\sin^2 \alpha'} - 1 \right)^{1/2} = \cot^2 \alpha'$$

Thus, the calculation of α_2 leads to $b_{\perp}$ which gives a length of line at the new height z_2 and the integration can be performed throughout the volume.

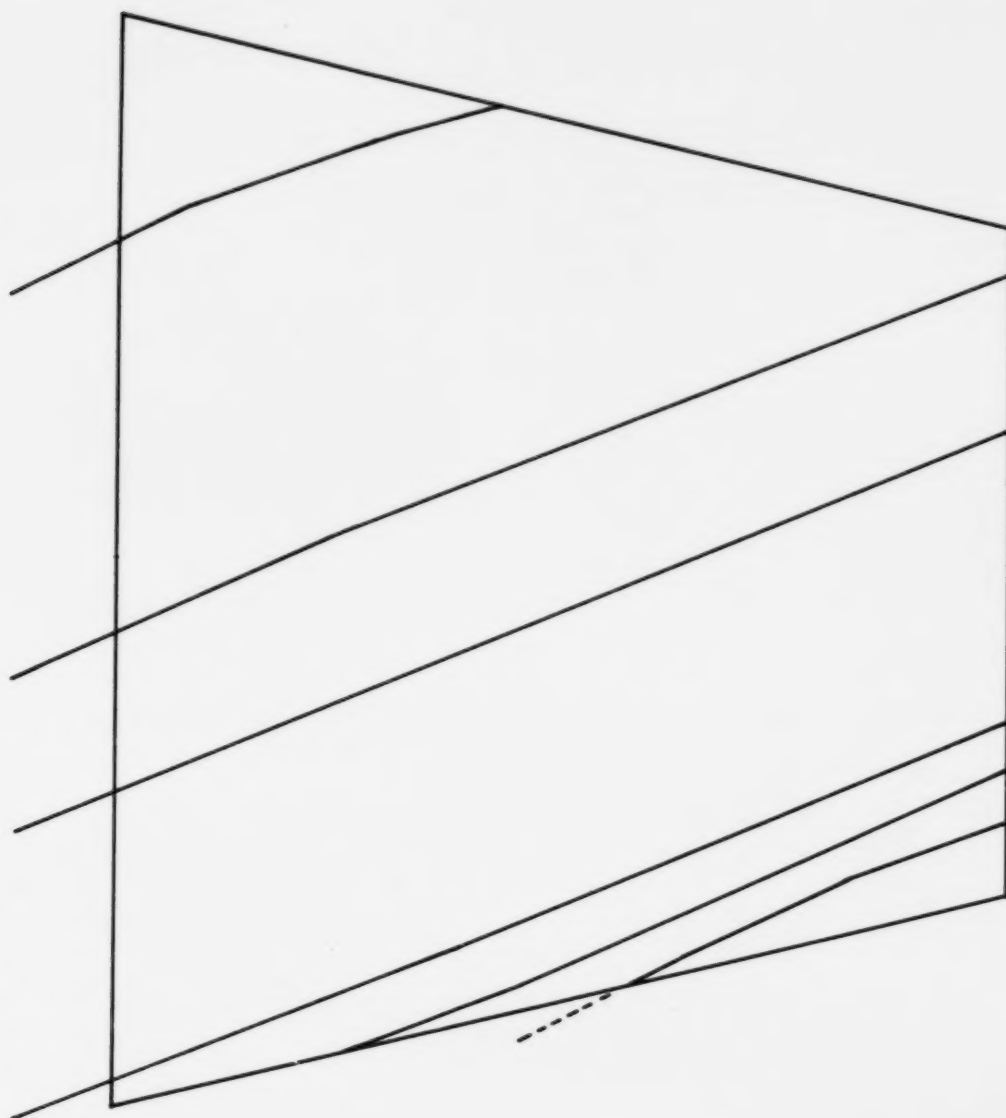


FIGURE 17 : THE CODOSS AS THEY GO THROUGH THE SCATTERING VOLUME. AS WIND SHEAR INCREASES, SO DOES CURVATURE.

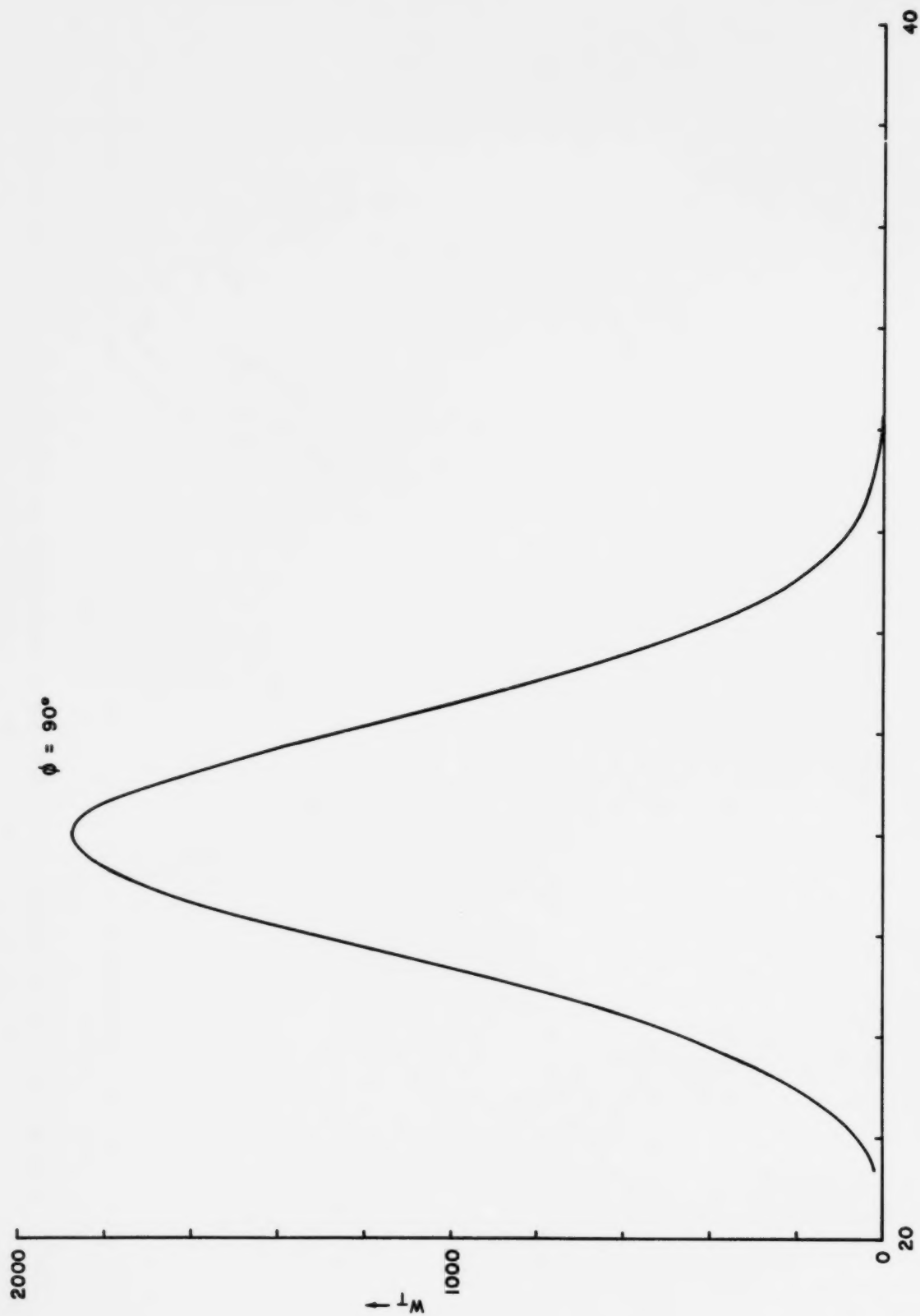


FIGURE 18. SPECTRUM FOR WIND SHEAR AND VERTICAL SOUNDER.

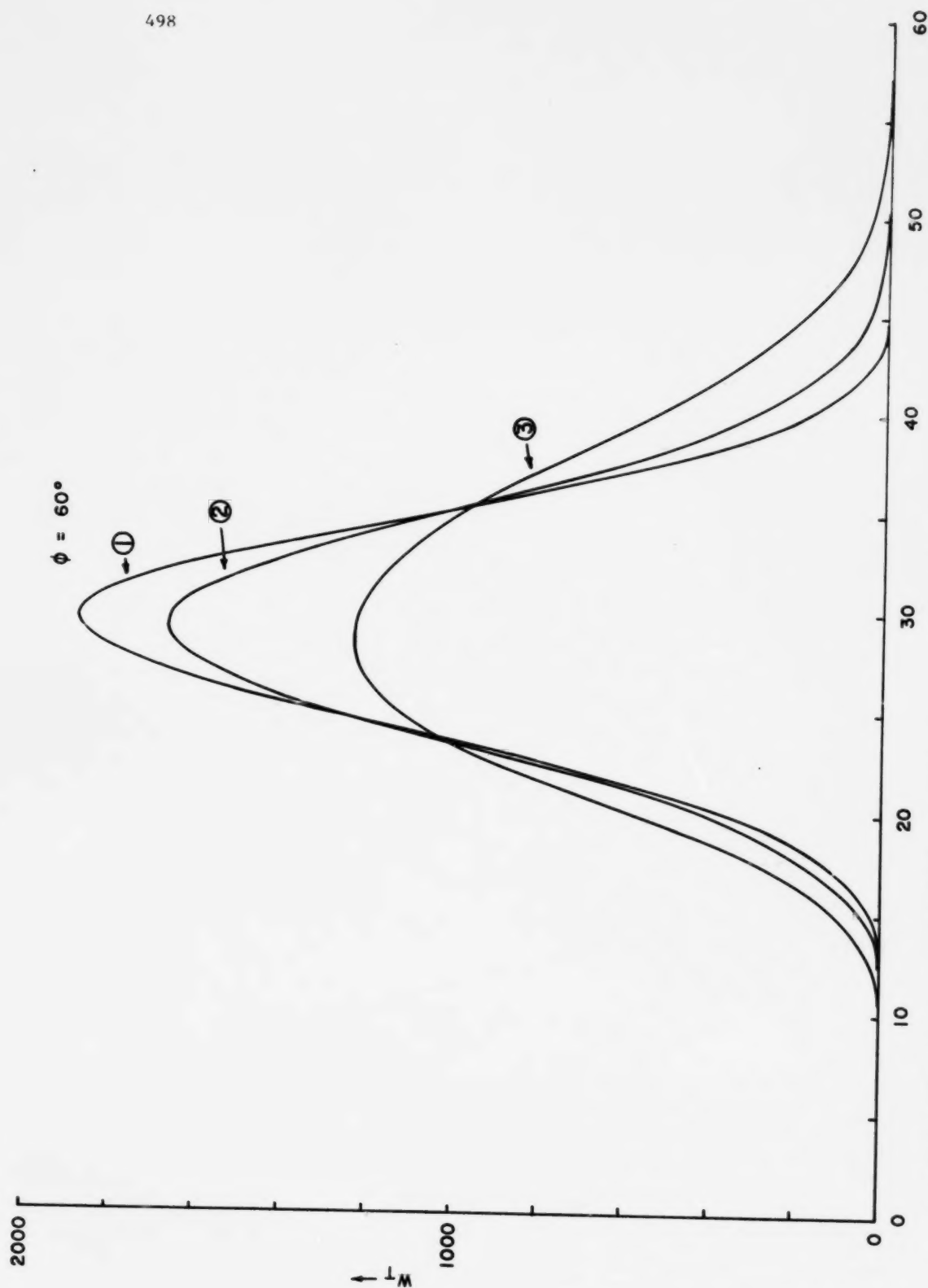


FIGURE 19 : WITH SOUNDER AT 60° FROM HORIZONTAL AND WIND SHEAR VARYING ① : $z_0 = 0$, $k = .02$, ② $z_0 = 400, k = .1$ ③ $z_0 = 450, k = .2$

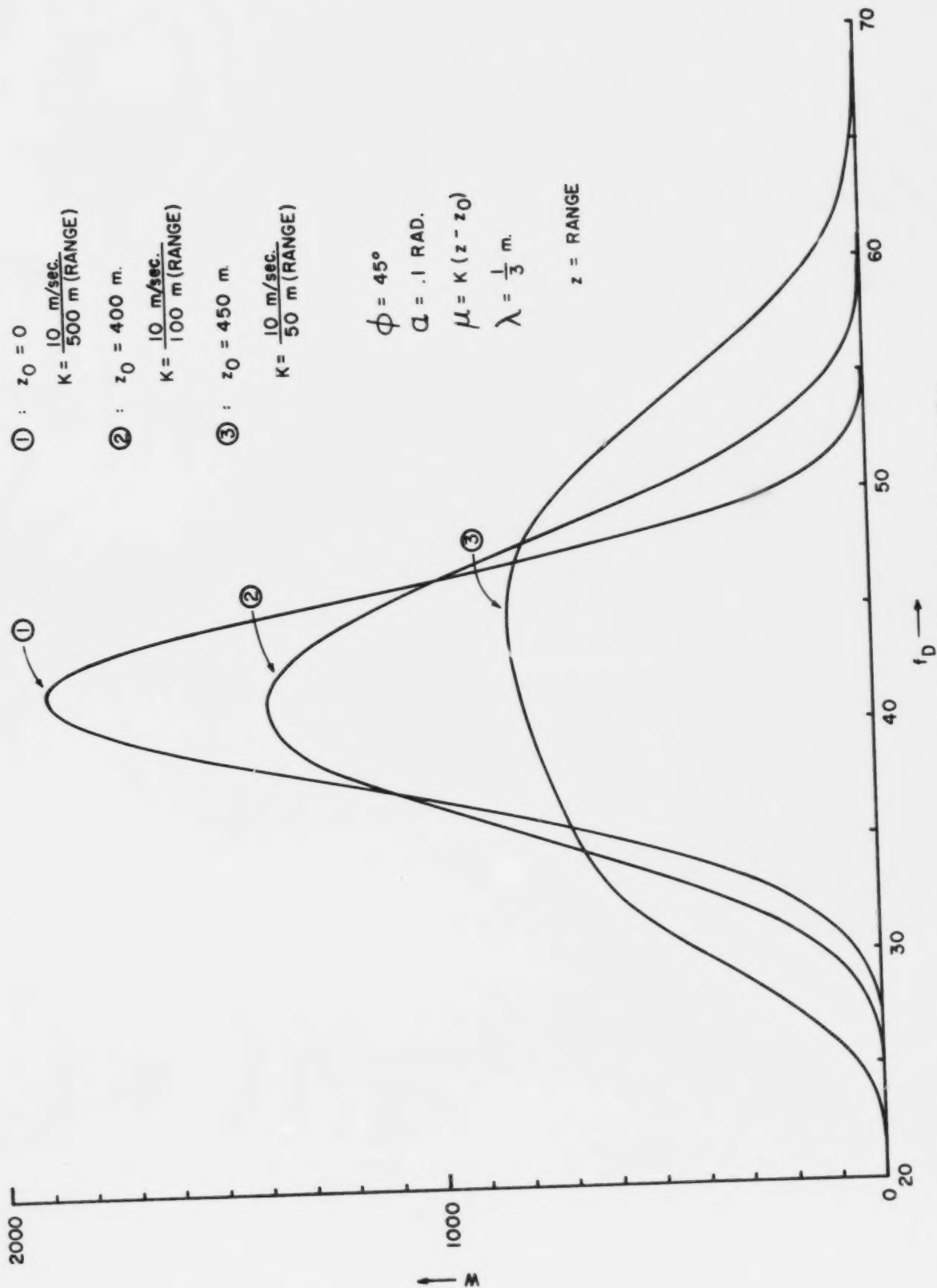


FIGURE 20: SPECTRUM FOR WIND SHEAR AND VERTICAL SOUNDER.

$\phi = 30^\circ$

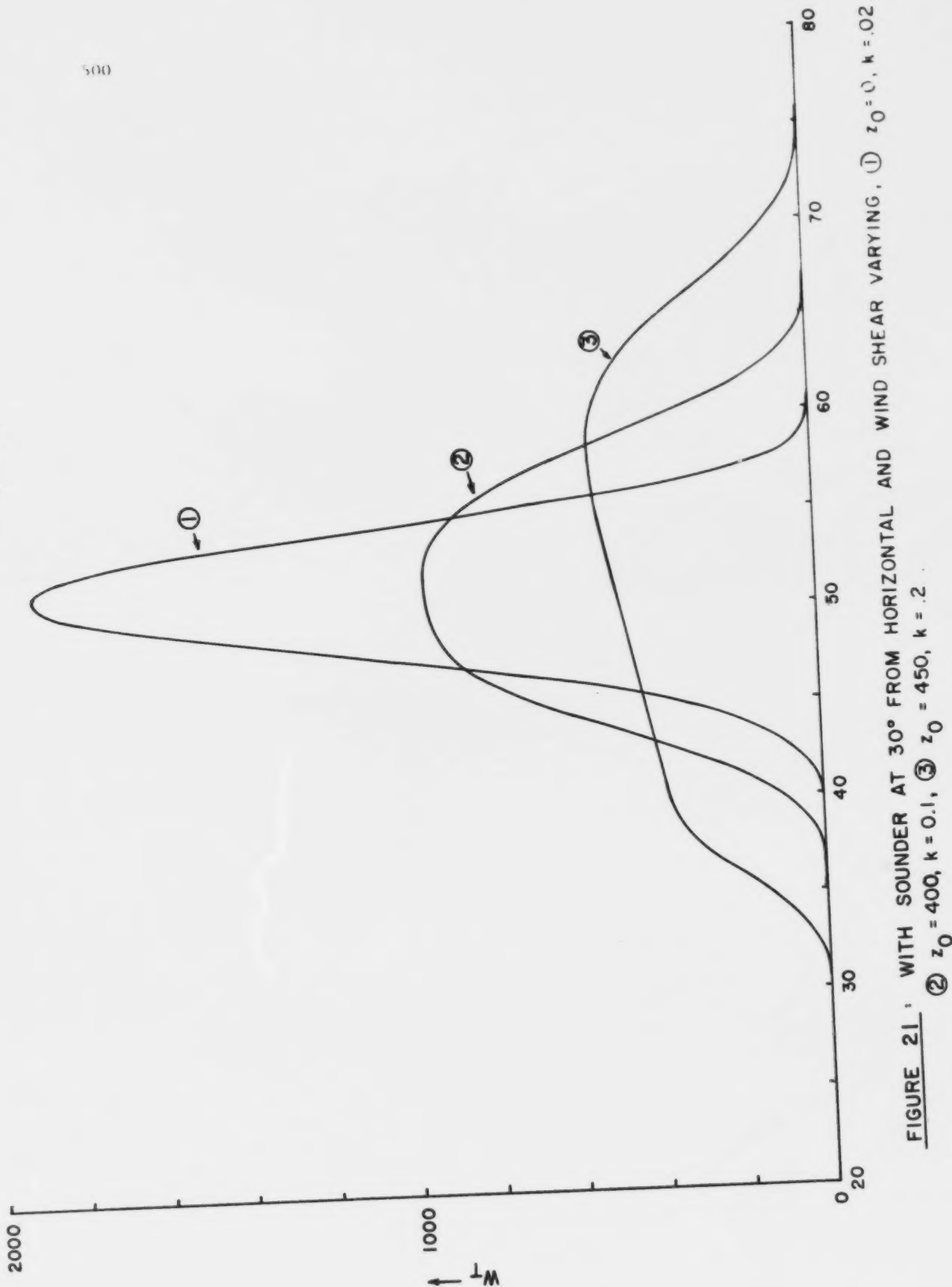


FIGURE 21: WITH SOUNDER AT 30° FROM HORIZONTAL AND WIND SHEAR VARYING, ① $z_0 = 0$, $k = .02$, ② $z_0 = 400$, $k = 0.1$, ③ $z_0 = 450$, $k = .2$.

Care must be taken when $\alpha' = \pm 3\alpha$. When $\alpha' > |3\alpha'|$, contributions are ignored. A sketch of the CODOSS as calculated in this manner is shown in Fig. (17). As can be seen, because of the wind shear, the CODOSS can enter and leave the defined volume as z increases. The exponential weighting causes the contribution at $\alpha' > |3\alpha'|$ to be negligible, however, care must be taken to count those lines which enter the volume above z_1 .

Figures (18) - (21) show the results of integrating in the previously discussed manner. The figures show the spectra at ϕ varying from 90° to 30° , each with varying wind shear and z . The three wind shear cases are picked in each case in a manner such that the wind speed at $z = 500$ m is 10 m/sec. This is done so that they may be compared to the no wind shear case which has wind speed 10 m/sec and the middle of its scattering volume at 500 m.

The wind shear case with $z_0 = 0$ and $k = .02$ is the closest to the no wind shear case and a comparison of the two yielded quite close results, which is only as it should be, but encouraging nonetheless.

As would be expected, as the shear is increased, there is a greater contribution to the wings of the spectrum and a decrease in the maximum height. In addition there is a slight shifting of the peak as the shear increases. This is due to the changing slope and curvature of the CODOSS with height and wind shear for at greater heights in the volume, the contributions near the beam center will be greater than at smaller heights.

The most noticeable effect, however is the occurrence of a linear portion of the spectrum near the peak with an increase of wind shear and/or decrease of ϕ . Thus far, the actual cause of this effect is unknown. Further study on this is now underway.

3.0 MONTE CARLO METHOD FOR EVALUATING ACDAR SCATTERING VOLUMES AND SYSTEM FUNCTIONS

R. J. Greenfield

Thomson and Coulter (1974) discussed the importance of careful analysis of the system function of an acdar system if sounding is to be used to obtain quantitative information on the state of the atmosphere. Expressions were given for evaluating such quantities as the scattered power arriving at the receiver and the volume common the source and receiver beams. To obtain numerical volumes for these quantities, it is necessary to carry out some sort of a volume integration. Their evaluation which was performed for uniformly weighted beams clearly showed how radically the system function normally changes with range.

To carry out the required integrations analytically is complex even for the constant weighted beam as discussed by Thomson and Coulter. In more realistic transmitter and receiver beam patterns, when, in addition, scattering loss, and angular dependent scattering coefficients are considered, an analytic solution for the evaluation of the system function will not normally be possible.

As a convenient alternative, a Monte Carlo evaluation of the numerical integration is under investigation. The desired integrals are of the form

$$I = \int_{\text{vol}} dV \cdot W(r) \quad (1)$$

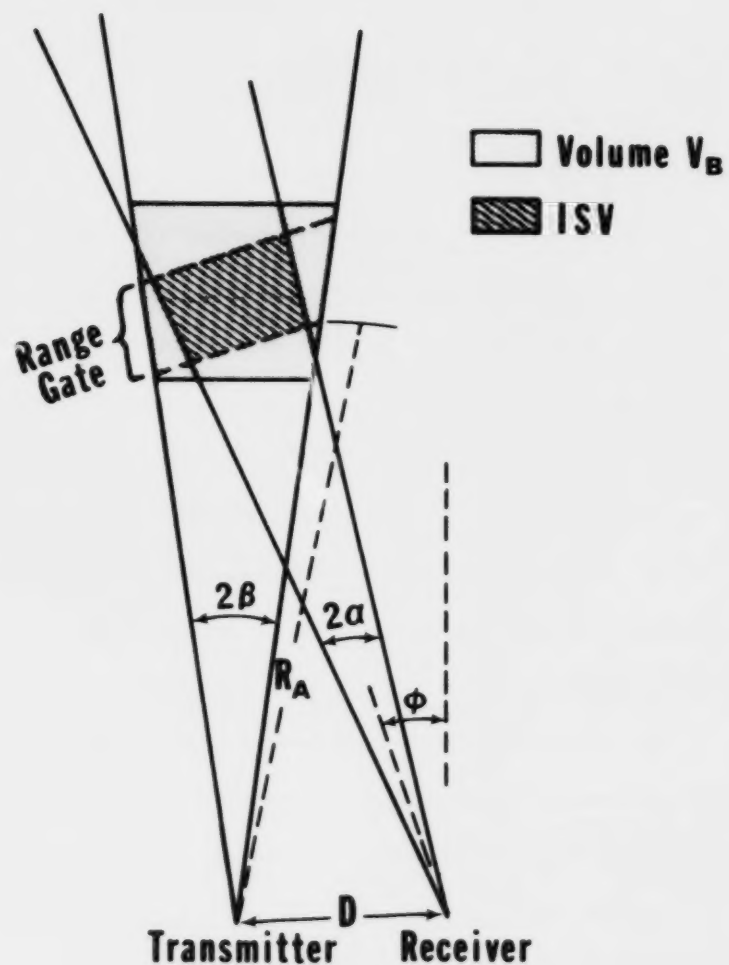


FIGURE 1 : INSTANTANEOUS SCATTERING VOLUME FOR A BISTATIC ACDA.

where $\vec{r}$ is the position vector and $W(\vec{r})$ is a position dependent weighting function.

As a specific example of such an integral we evaluate the instantaneous scattering volume (ISV), the volume within a range gate, of a bistatic radar system. The ISV for a pulse of length $\ell = C \cdot \tau$ is the volume common to the transmitter and receiver beams which contributes to the energy arriving at the receiver at some instant of time. Here τ is the time duration of the pulse, and C is sound speed. Thus for a point to be in the ISV, as well as being in both beams, the travel time $T = (R_T + R_R)/C$ must obey $2 \cdot R_A \leq C \cdot T < 2 \cdot R_A + \ell$. Here R_A is the range to the start of the scattering volume as shown in Figure 1; R_T and R_R are the range from the point to, respectively, the transmitter and receiver.

To calculate the instantaneous scattering volume by the Monte Carlo method consider

$$A \equiv \frac{\int_{V_B} W(\vec{r}) dV}{\int_{V_B} dV} \quad (2)$$

The value of A is the average of $W(\vec{r})$ over the volume V_B . For the calculation of the ISV, $W(\vec{r})$ is 1 for points in the ISV and 0 elsewhere. Thus A is the ratio of the ISV to V_B . We take as V_B the volume

between two planes normal to the transmitter axis. The position of the planes is chosen large enough to contain the whole of the instantaneous scattering volume. The value of A is found by randomly generating points in the volume V_B . As the number of points goes to infinity the fraction of the random points for which $W(\vec{r}) = 1$ approaches A . Even for a finite number of random points, we obtain a good estimate of A . The volume of V_B is readily calculated analytically since it is the volume of a truncated cone. Thus equation 2 can be used to estimate the ISV.

The results of the Monte Carlo calculation of the ISV were compared to analytic results given by Thomson and Coulter. Comparisons are shown in figures 2 and 3. In figure 2, $\tau = 80$ ms, $C = 320$ m/s, $D = 100$ ms, the transmitter beam width, $\beta = 2^\circ$, and the receiver beam width, $\alpha = 1^\circ$. The transmitter axis is vertical, and the receiver tilted at $\phi = 10^\circ$ from the vertical, towards the transmitter. The calculation was made generating 3000 random points and required approximately 15 seconds of computer time (System 360). We consider the accuracy of the Monte Carlo results to be satisfactory.

Also shown on figure 2 is a calculation of the ISV when the responses of transmitter and receiver beams are dependent on the angle from the beam axes (non-uniform beam weighting functions). Antenna pattern power factors of $\exp \{- 50 \cdot \frac{\pi}{180} \cdot \theta_R \}$ and $\exp \{- 25 \cdot \frac{\pi}{180} \cdot \theta_T \}$

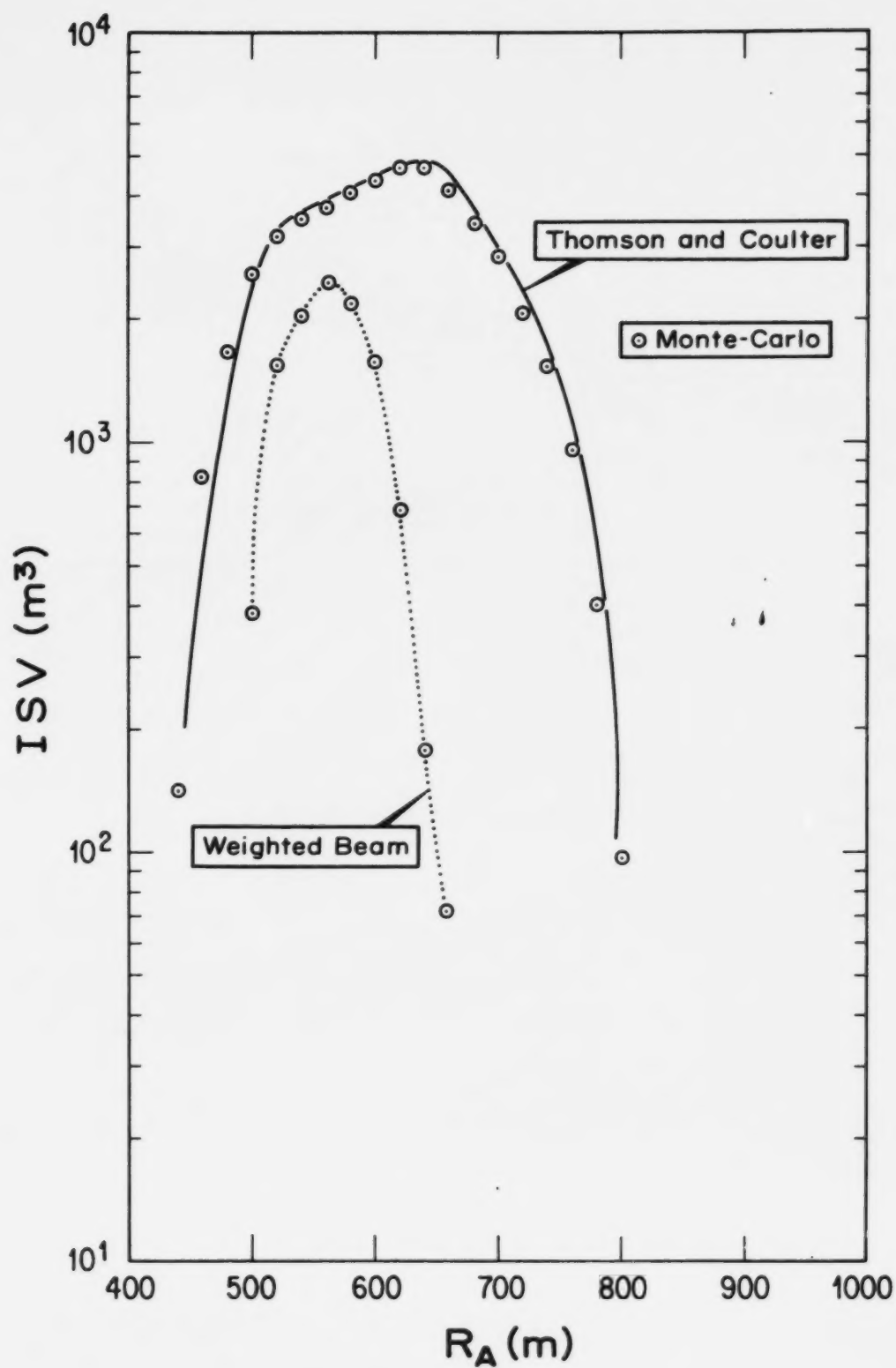


FIGURE 2: SYSTEM FUNCTION AS A FUNCTION OF RANGE. COMPARISON OF ANALYTIC AND MONTE - CARLO SCHEMES.

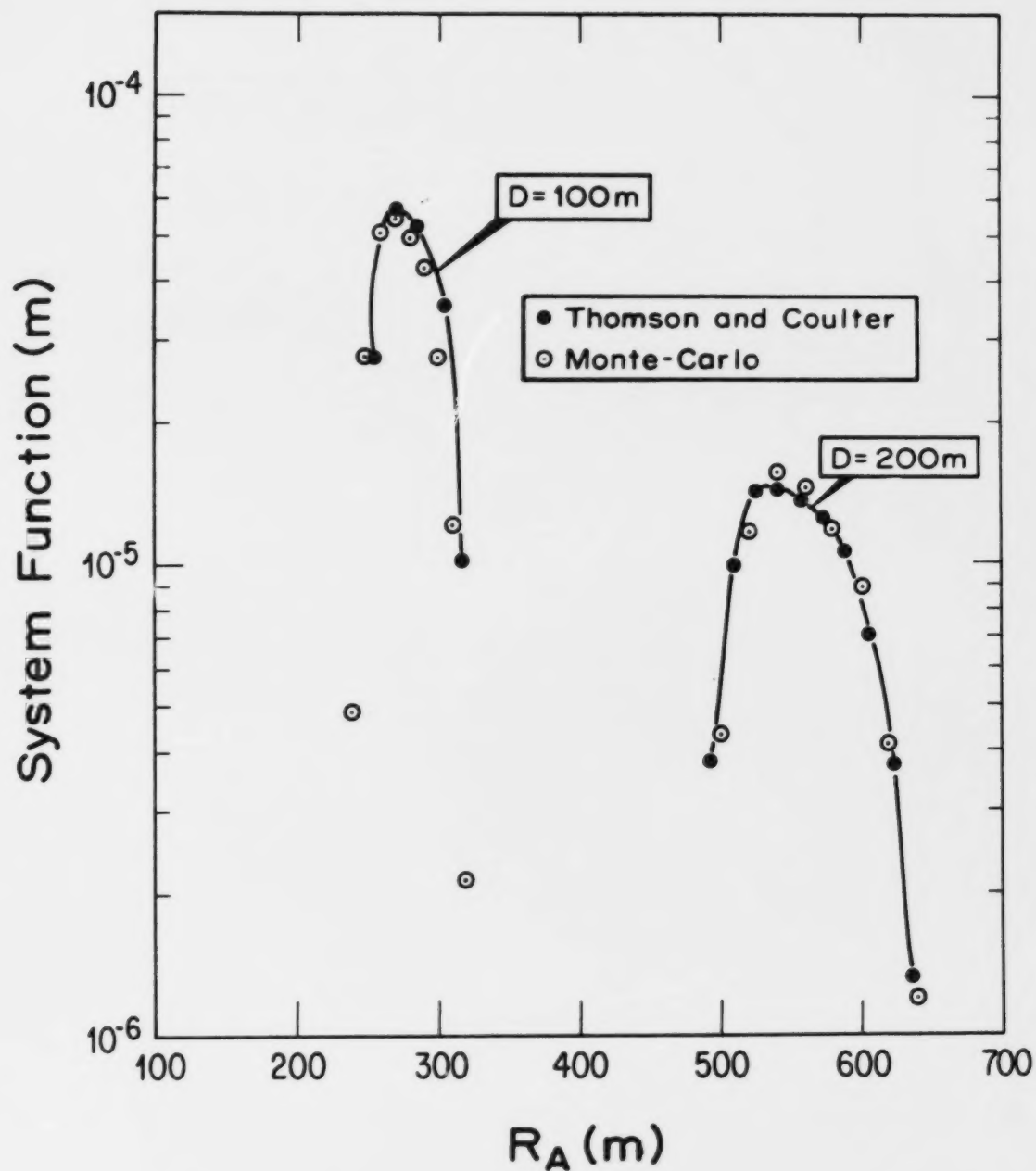


FIGURE 3: SYSTEM FUNCTION AS A FUNCTION OF RANGE. COMPARISON OF ANALYTIC AND MONTE - CARLO SCHEMES.

have been applied. Here Θ_R and Θ_T give the angle, respectively, from the receiver and transmitter axes. All other parameters are the same as in the previous example. The antenna pattern has, of course, an effect equivalent to narrowing the beam widths. This calculation of the ISV for the beam weighted bistatic configuration would be extremely difficult by analytic methods.

An additional calculation made to further compare Monte Carlo results for the system functions with analytic results of Thomson and Coulter is shown in figure 3. For these calculations $\alpha = 1^\circ$, $\beta = 2^\circ$, $\tau = 100$ ms, $\phi = 20^\circ$, and the D values are given on the figure. The expression for $W(\vec{r})$ for the system function is $\frac{1}{\Omega_T R_T^2 R_R^2}$ when the

point is in the ISV and 0 elsewhere. This $W(\vec{r})$ leads to the system function given by Thomson and Coulter. Ω_T is the solid angle of the receiver beam.

4.0 MEASUREMENTS OF SOUND REFRACTIVELY TRANSMITTED IN THE PLANETARY BOUNDARY LAYER

M. Teufel, M.S. Thesis Research in Progress

4.1 Introduction

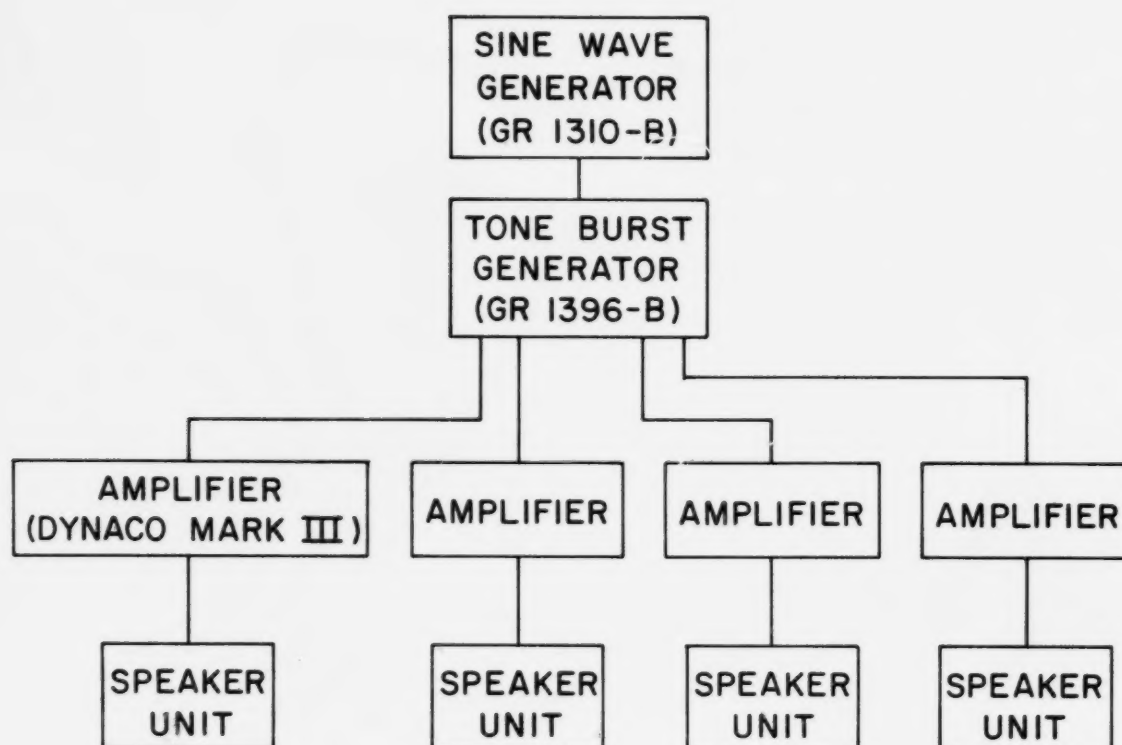
A bistatic acoustic probing system for studying temperature inversions within the planetary boundary layer (PBL) has been constructed and used to transmit sound to receivers located at distances ranging from a few to more than 10 km. The system consists, basically, of a 200 Hz acoustic transmitter, a fixed receiver station at which a micro-microbarograph is also located, and a second truck-mounted mobile acoustic receiver.

The system is being used in two types of studies. The first is to evaluate a scheme (Greenfield et al, 1974) for estimating temperature gradients in PBL inversions. The second study consists of an examination of the statistical properties of the fluctuations in the received acoustic signal level.

4.2 System Description

The transmitter consists of a 200 Hz CW source, and a variable tone burst generator which drives a series of 4 power amplifiers (Fig. 1). The 200 Hz operating frequency was chosen because of its relatively low attenuation under expected relative humidity and temperature conditions. In order to be able to vary the antenna beamwidth, a "phased array" transmitter configuration was chosen (Fig. 2). Each power (60 CW watts)

FIGURE 1 : TRANSMITTER DIAGRAM



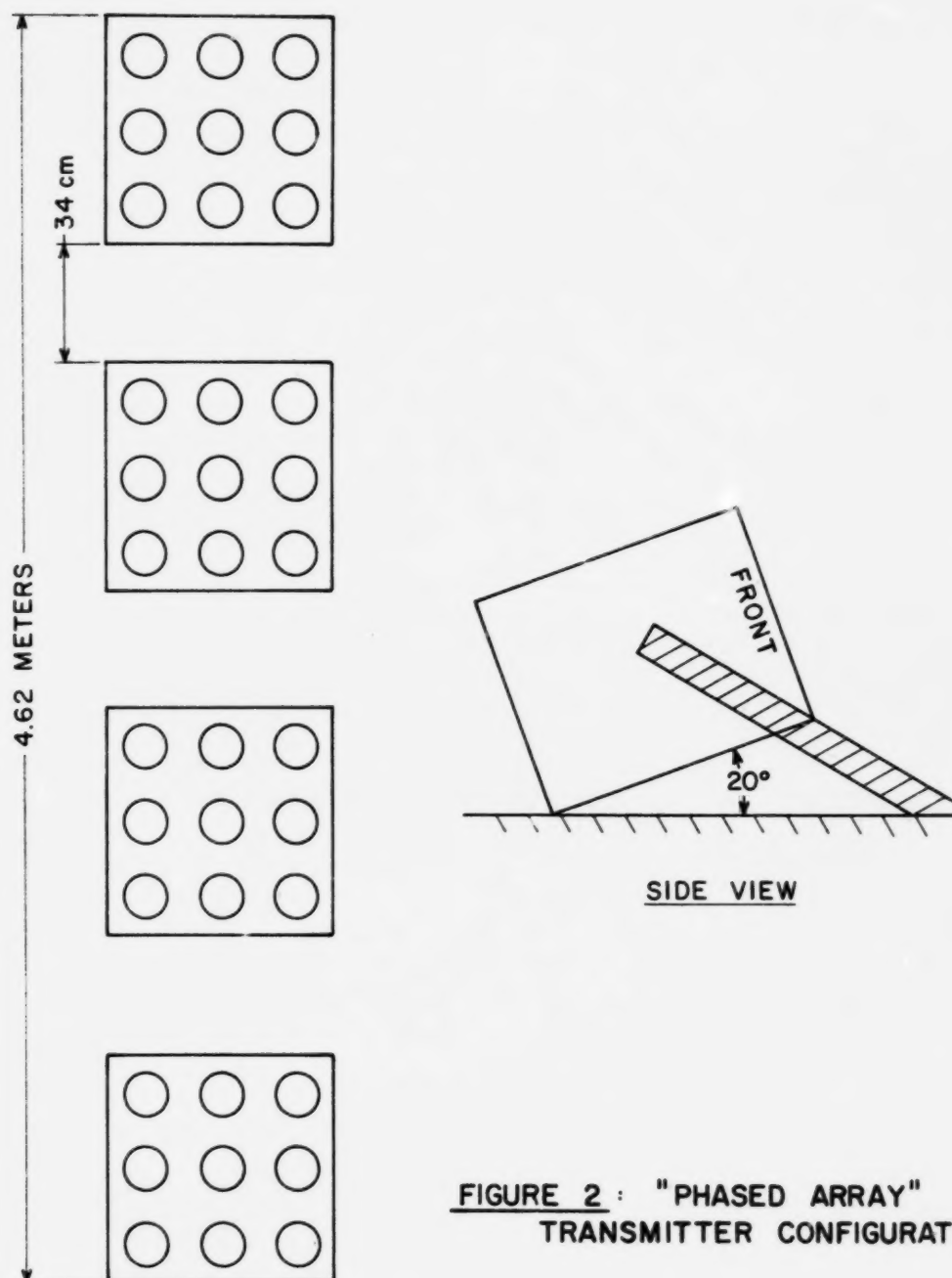
REFRACTION CONFIGURATION

FIGURE 2 : "PHASED ARRAY"
TRANSMITTER CONFIGURATION

amplifier drives a separate speaker enclosure. Each enclosure is equipped with nine 8" woofers. The separation of the approximately 1 m^3 enclosures may be varied to adjust the acoustic beamwidth from essentially that of an isotropic source to one of only a few degrees beamwidth. Measurements of the total transmitted acoustic power (≈ 12 watts) show the emitted patterns are in agreement with theory, at least to within the experimental error resulting from ground reflections. Fig. 3 shows the emitted pattern for three different power levels superimposed with the theoretical pattern for the speaker enclosure configuration previously shown in Fig. 2.

One receiving unit is van mounted. Since a directional antenna at 200 Hz cannot be made readily portable, an "omidirectional" microphone is used as an antenna-receiver. The received signal is preamplified, filtered in an active bandpass filter (CF = 200 Hz, BW = 10 Hz) and both the filtered and unfiltered outputs recorded on a multi-channel analog tape recorder (see Fig. 4). The filtered signal is also envelope detected, averaged on an integrating RMS volt meter and then displayed as "signal strength" on a strip chart recorder.

Fig. 5 is an example of typical unfiltered and filtered signals obtained at approximately 5:30 a.m. on the morning of September 13, 1974 at a range of 3.6 km.

In addition to the van-mounted receiver, a second acoustic receiver was placed at a fixed base station (University Park Airport) 4.7 km from the transmitter. This was done to allow continuous monitoring of the signal as atmospheric conditions changed. A recording micro-microbarograph was constructed and positioned at this station.

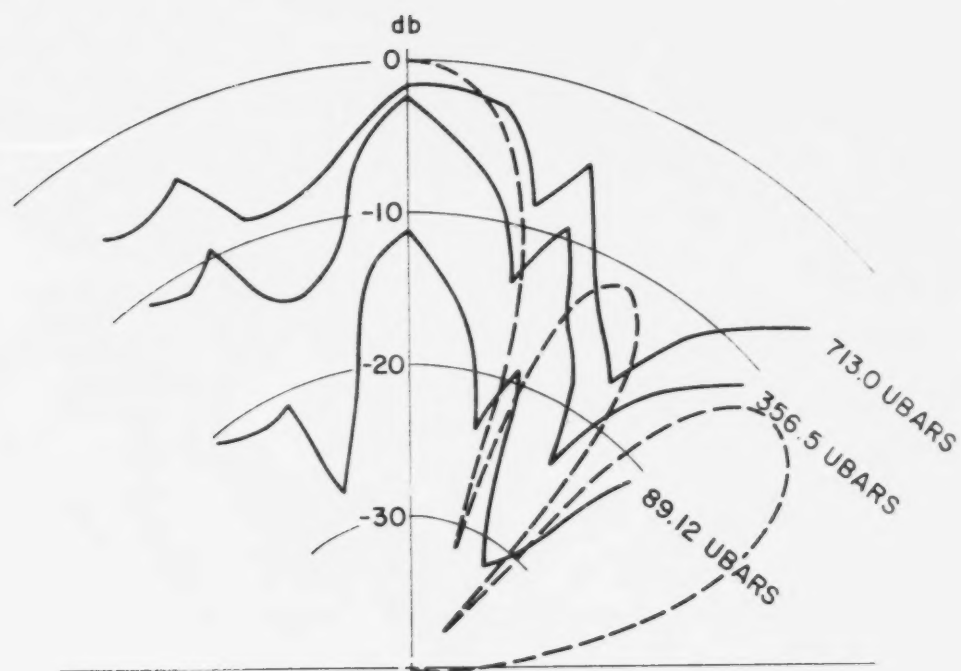
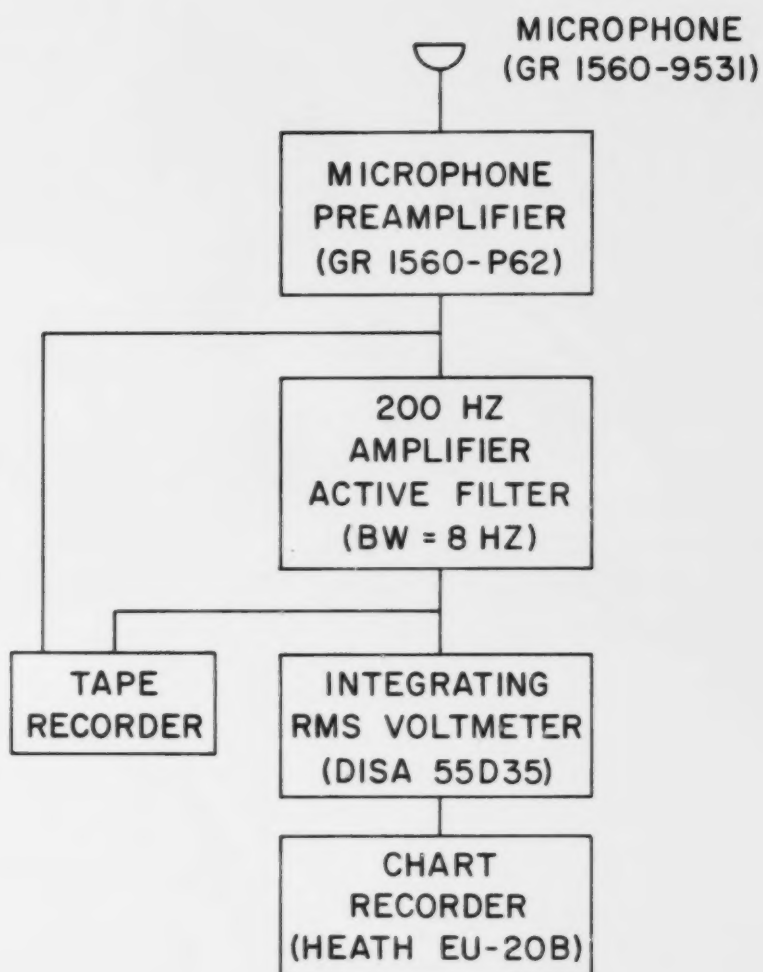


FIGURE 3: COMPARISON OF MEASURED AND
THEORETICAL BEAM PATTERNS

RECEIVER DIAGRAMFIGURE 4 : RECEIVER BLOCK DIAGRAM

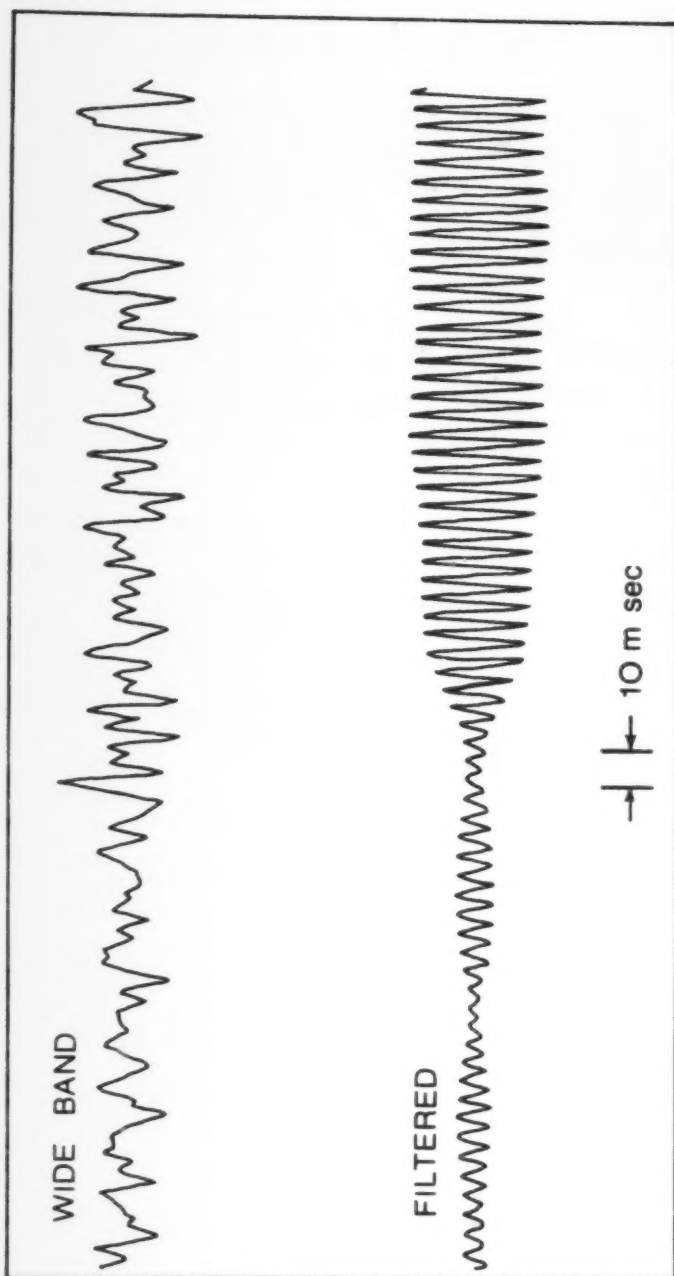


FIGURE 5: COMPARISON OF RAW AND FILTERED RECEIVED SIGNALS.

4.3 Measurement of Inversion Layer Temperature Gradients

A method for measuring the temperature gradient, T_2' , in an elevated inversion layer has been developed. A paper describing the method has been accepted for publication in the Journal of Geophysical Research and a preprint is included as Section 4 of this report.

Briefly, the method requires two quantities to be measured. First, the height of the base of the inversion layer must be determined. This will be done with a monostatic sounding system which is presently being constructed and tested. The second quantity needed to resolve T_2' is the distance to the caustic. It can be determined either by a high sound level or by the smallest distance at which sound is detected.

For an elevated inversion layer sound rays transmitted at a low angle to the vertical will initially bend upward, then return to the surface. The caustic is then the minimum distance at which the sound rays will return (distances less than the minimum will be referred to as the zone of silence).

Preliminary measurements have been made to determine the ability to locate the caustic. The following are two examples of these measurements.

Data was collected on July 7, 1974 with the fixed acoustic receiver at the airport and the van-mounted receiver roving from location to location. Fig. 6 shows several sections of the record from the truck mounted receiver. From this data a plot (Fig. 7) of maximum amplitude versus range was made. The amplitude decreases with increasing range from the airport. However, the amplitude is lower at the SA station than at the airport.

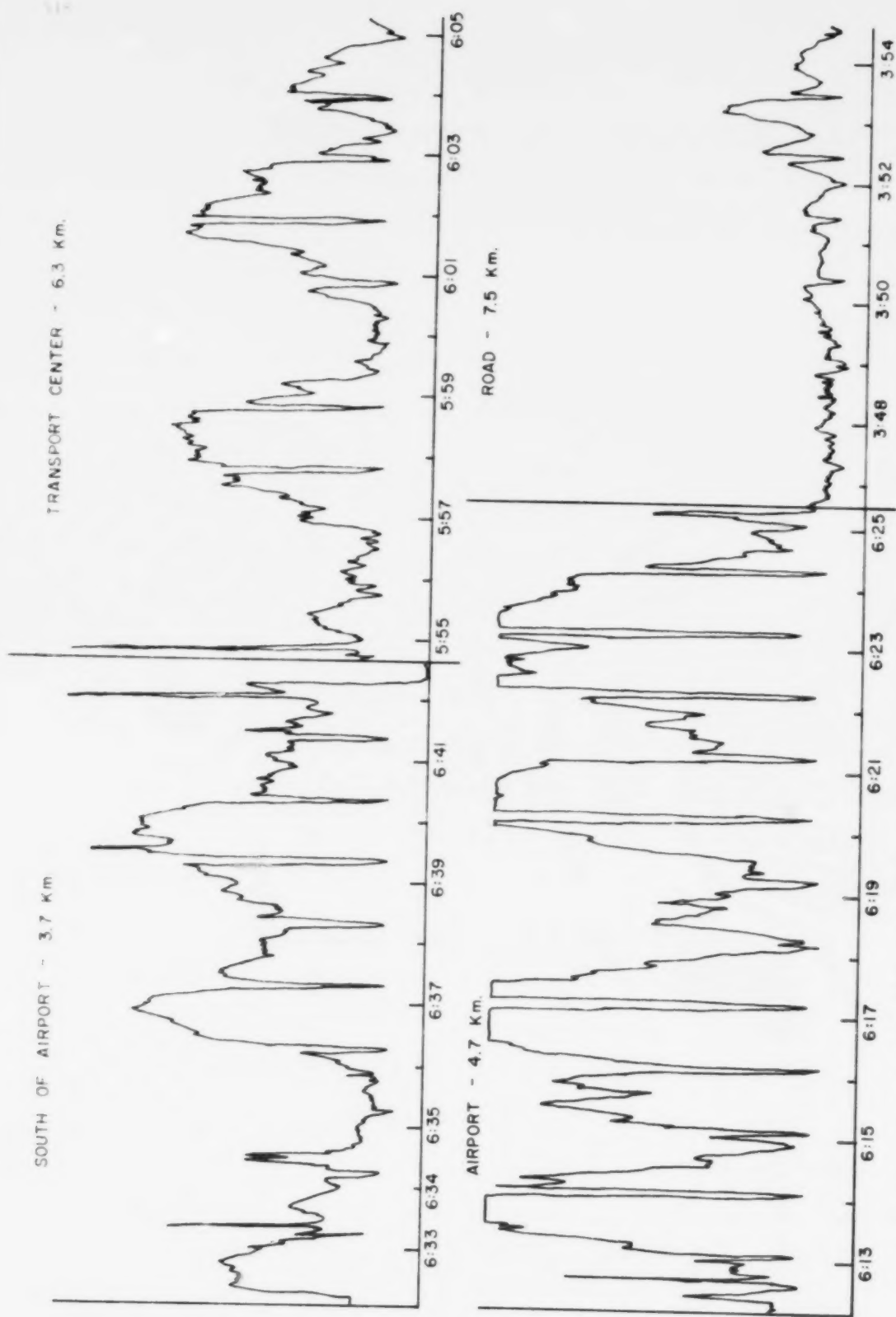


FIGURE 6 : SOUND LEVELS MEASURED AT VARIOUS RANGES ON MORNING OF 7 JULY 1974

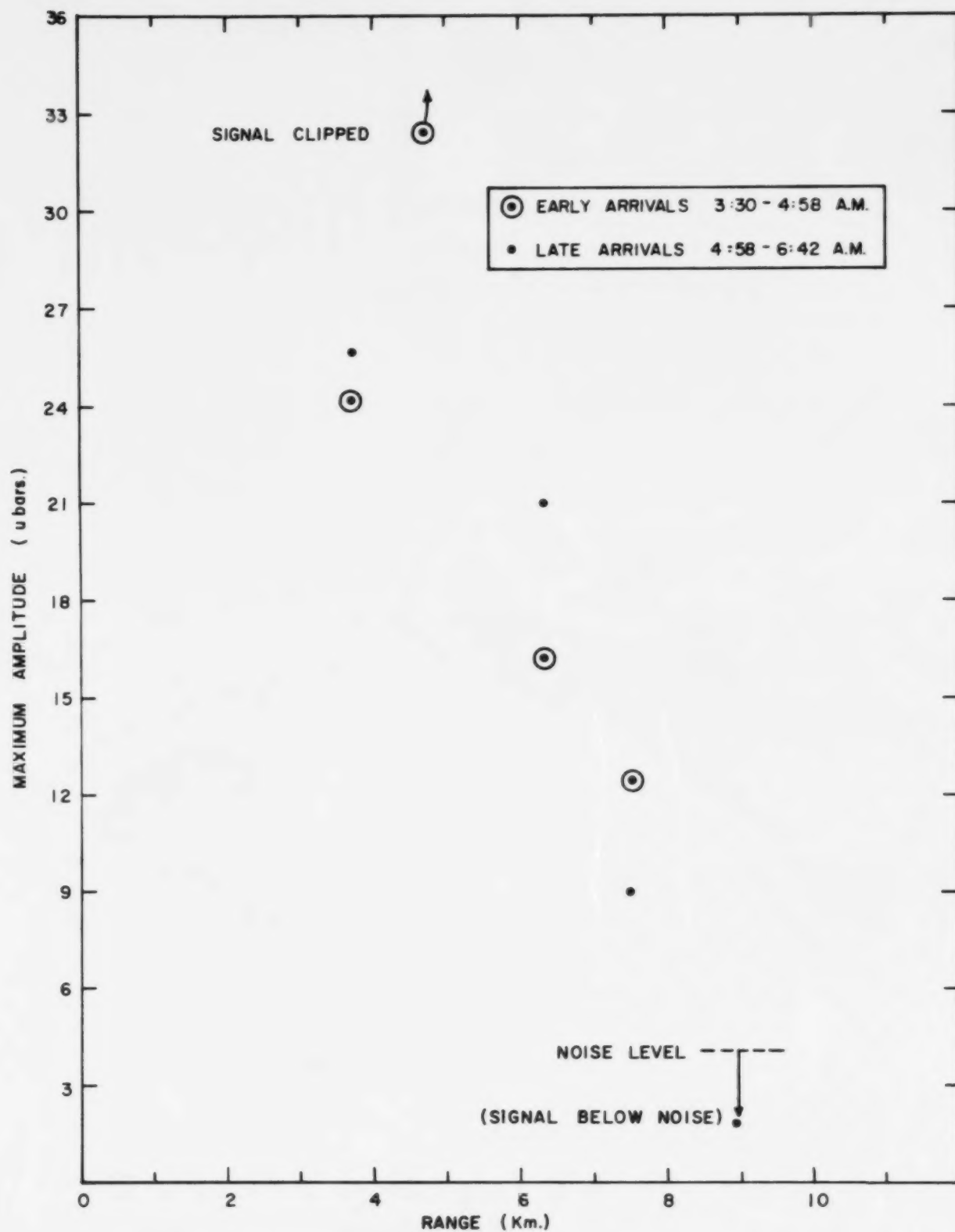


FIGURE 7: MAXIMUM AMPLITUDE VS. RANGE.

Thus the amplitude is not a monotonically decreasing function of range. We believe that the lower sound level at the SA station was due to scattered energy (Wiener and Keast, 1959) while the arrivals from the airport outward were actual refracted arrivals. Thus the zone of silence ends somewhere between the SA and airport stations.

Data taken on August 21, 1974 may be an example of arrivals from a raised inversion. Fig. 8 shows the sounder record at the TC station (6.4 km). The first section was received at approximately 6:00 am and has a peak amplitude of 31.7 ubars. The second section received at 6:35 am shows a greatly reduced signal level, 4.4 ubars which is practically buried in noise. The signal amplitude at the TC station decreased considerably as the rising sun destroyed the inversion layer.

After sunrise, the sounder record at the fixed airport station (4.7 km) was also reduced to a level below the noise.

These two examples suggest that the zone of silence from the source to the caustic distance has been observed. When the monostatic sounder is in operation later this fall, it will be possible to much better establish the existence and the height of the inversion layer. Thus, we will be more confident of the zone of silence observations.

4.4 Fluctuations of Signal Levels and Possible Association with Atmospheric Gravity Wave Motions

In the course of our experimentation with the long baseline acoustic sounder we have regularly observed apparently periodic fluctuations in the signal amplitude (Figures 6 and 8). The fluctuations appear to have periods

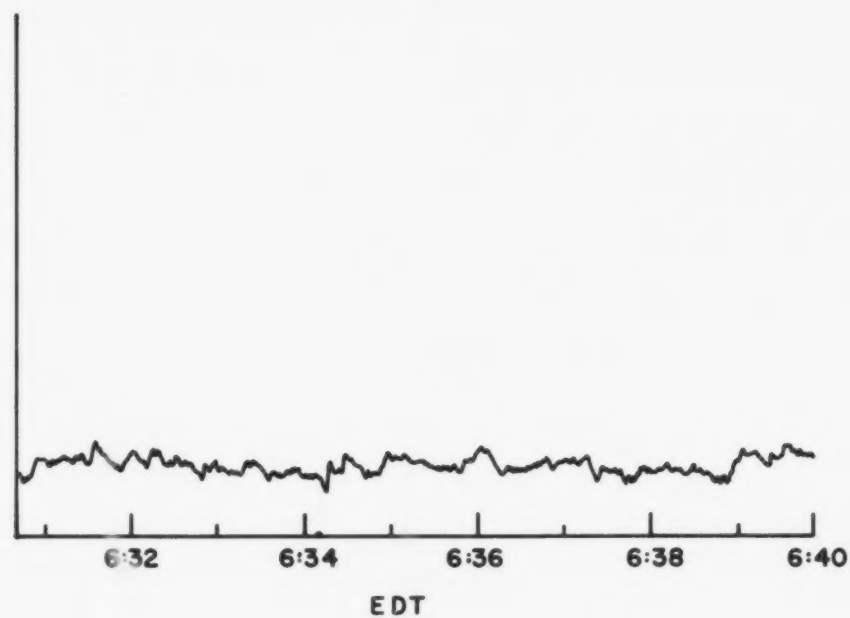
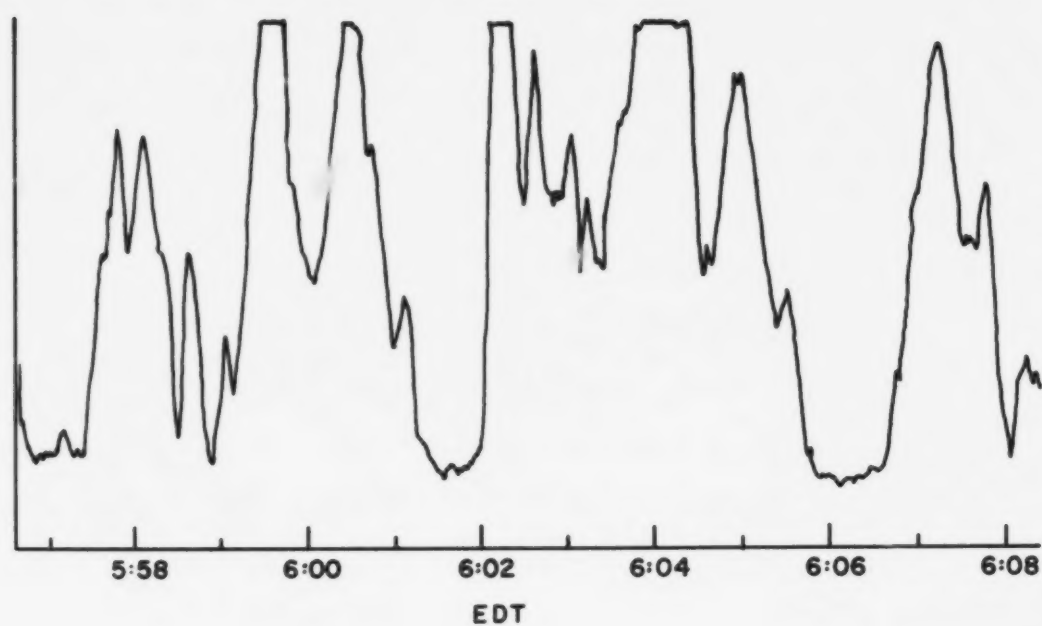


FIGURE 8: TRANSPORT CENTER RECORD ON MORNING OF
21 AUGUST 1974.

on the order of minutes and over extended periods, a sinusoidal pattern with periods varying from 15 to 30 minutes is also frequently evident. It should also be noted that most of the data has been collected on mornings when there were clear skies overnight and winds were calm (conditions commonly associated with high pressure systems).

For refractively propagated signals, changes in signal strength are due to one of two causes. The first possibility is that the sound reaching the receiver follows a single ray path. Then the amplitude fluctuations simply reflect changes in the geometric spreading of the ray. The second possibility is that the amplitude fluctuations are caused by some type of multipath phenomenon. Energy arrives along two or more ray paths, and gives a large signal when the individual rays tend to be in phase and a low level signal when the individual rays destructively interfere.

The above observations led us to investigate the possibility that the fluctuations might be associated with gravity waves. Observed (e.g., Gossard, E. E. and W. H. Munk, 1954) for many years using microbarographs, these waves have periods of approximately 5 - 30 minutes and amplitudes on the order of tenths of millibars. In order to confirm our hypothesis, a micro-microbarograph was constructed earlier this summer and located at the airport station.

Figure 9 shows a portion of one barograph record received in the early hours of the morning of August 1, 1974. The sinusoidal character of the gravity waves is obvious; the waves have a period of approximately 45 minutes and a fairly uniform amplitude of .34 mbar. Although sound data were

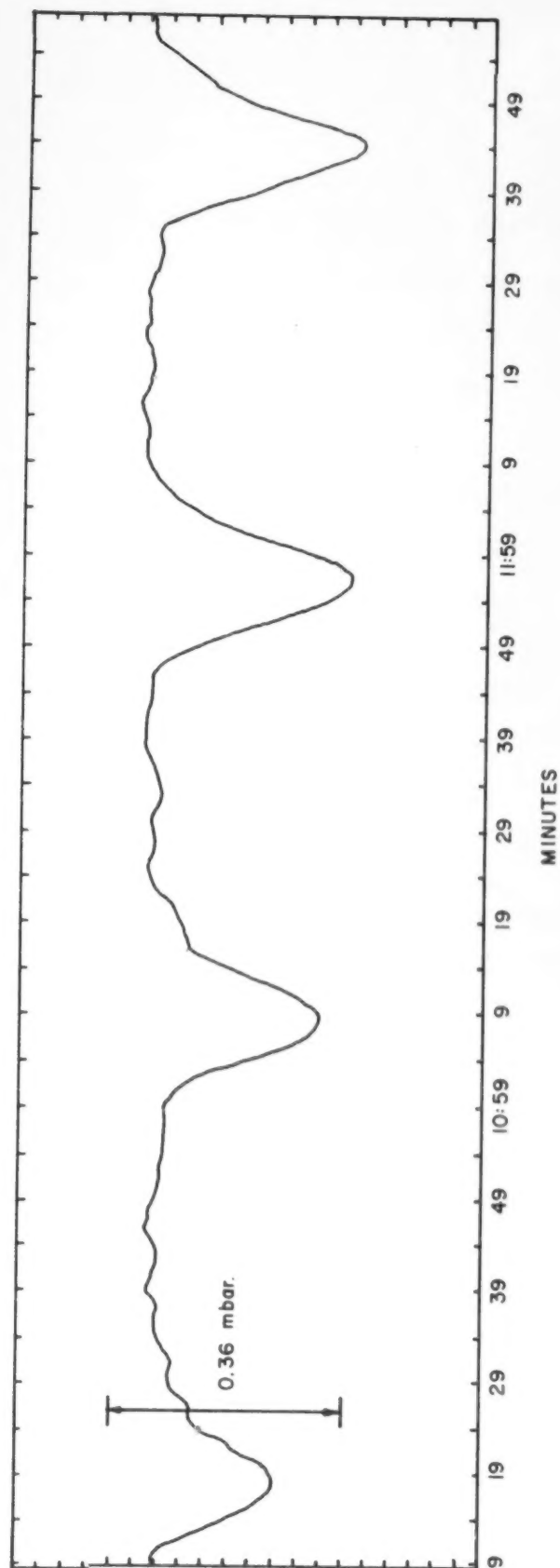


FIGURE 9: ELECTRONIC MICROBAROGRAPH TRACE FROM MORNING OF 1 AUGUST 1974.

also obtained, no obvious correlations between the sound level and pressure fluctuations were evident.

Both the barograph and sounder (fixed station) data of July 13, 1974, are shown on a reduced time scale in Fig. 10. On this particular morning, the signal to noise level for the acoustic record was quite high (≈ 10). Again, no obvious correlation is evident.

Work is presently underway to objectively analyze the fluctuation data. Power spectra are being computed for the sounder microbarograph records. Further, data will be taken to establish the spacial correlation properties of the sounder amplitude fluctuations.

Modeling of signal amplitude based on ray tracing in atmospheric models which are not horizontally layered is also being conducted. Such models may be used to represent layered structure perturbed by a gravity wave. The modeling of signal amplitudes will examine both geometric spreading and multipath interference effects.

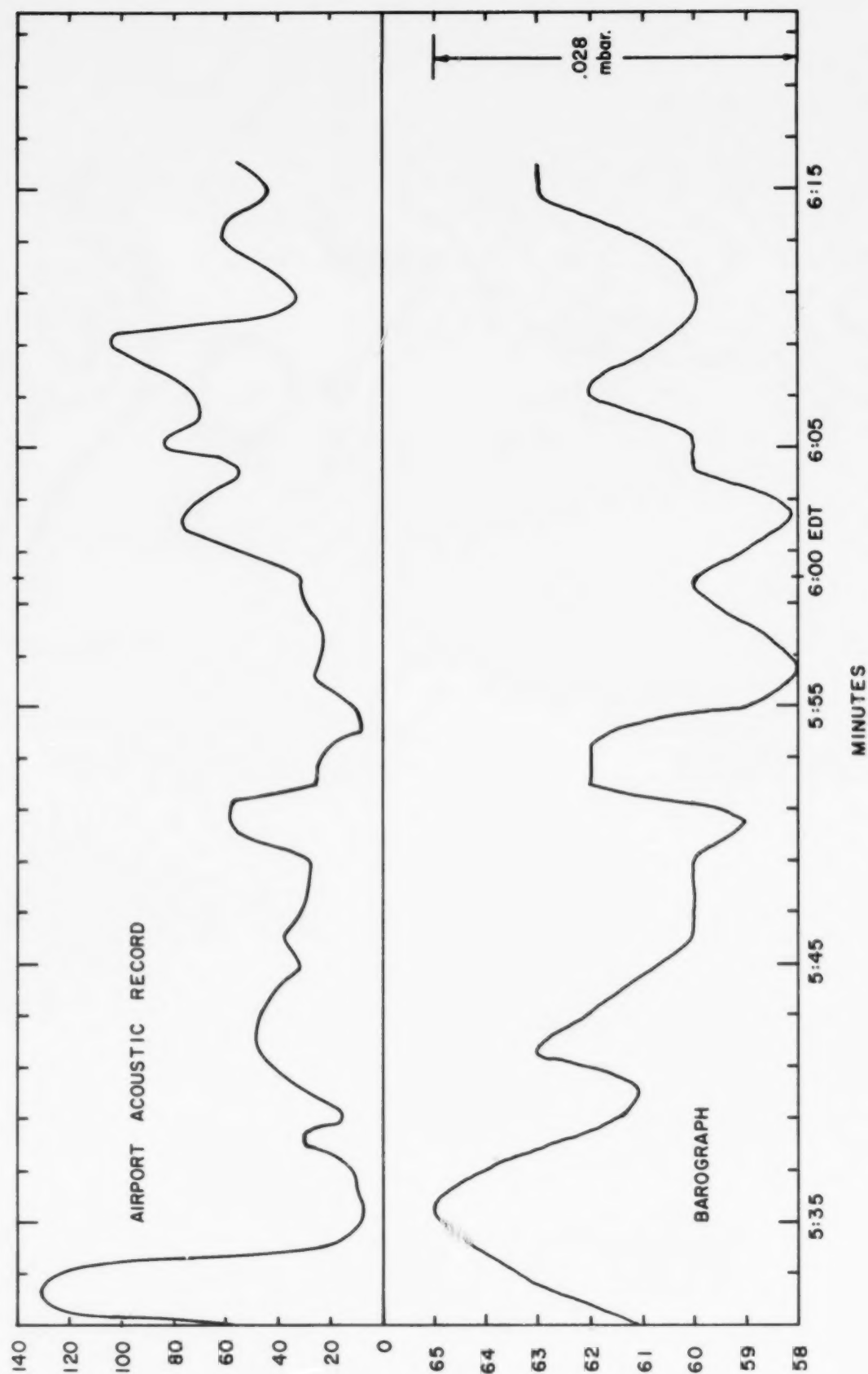


FIGURE 10 : COMPARISON OF SOUNDER AND BAROGRAPH OBSERVATION FOR MORNING OF 13 JULY 1974.

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- Wiener, F. M. and D. N. Keast; Experimental Study of the Propagation of Sound Over Ground, J. Acoust. Soc. Am., 31, 724-733, 1959.
- Gossard, E. E. and W. H. Munk; On Gravity Waves in the Atmosphere, J. Meteor., 11, 259-269, 1954.

5.0 Temperature Profile Measurements in Inversions
from Refractive Transmission of Sound

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Abstract

A method is described for estimating temperature profiles in the lower troposphere during conditions including a surface-based or elevated inversion layer. The method uses acoustic energy transmitted over paths on the order of ten kilometers in length. Measurements are made at approximately one kilometer intervals extending radially outward from the transmitter. The vertical temperature profile is modeled as two constant temperature gradient layers. The first layer extending from the surface to height H_1 has a temperature gradient T_1' (usually negative upward). The second layer temperature gradient T_2' is strongly positive upward. For temperature profiles of this type, ray paths arrive with a high intensity at a caustic, and no rays return to earth between the source and the caustic. The method requires that H_1 be determined by some other means such as vertical radar sounding. T_1' and T_2' are then simultaneously determined by measuring the range to the caustic and the wave propagation time. Even if the propagation time can not be measured, useful estimates of T_2' can be obtained from observations of H_1 and the caustic distance. For a ground-based inversion no caustic occurs. However, the temperature profile can be determined by measuring the wave propagation time. Since horizontal wind shear produces the same effect on ray paths as a vertical temperature gradient, the proposed method obtains the sum of the effects of the wind shear and the temperature gradient. In conditions including significant wind shear, corrections for it must be made.

I. Introduction

Atmospheric refraction of sound has been recognized for more than fifty years to be the consequence of particular atmospheric temperature and wind profiles. In fact, some of the earliest estimates of stratospheric temperatures were made using explosion sound observations. Recently, the development of various acdar systems has revived interest in using acoustic signals for, in particular, low-level atmospheric sounding. Observations of planetary boundary layer structure, winds, gravity waves and turbulence have been made by a number of research groups (see, e.g.: McAllister, 1968; Little, 1969; Beran et al., 1971; Beran and Clifford, 1972; Cronenwett et al., 1972; Hooke et al., 1973; and Bean et al., 1973).

The amplitude of received acdar signals depends upon the intensity of scattering or partial reflection of sound in regions of turbulent temperature and wind fluctuations. The altitude of a scattering region is determined using the elapsed signal travel time and atmospheric velocities are inferred from the properties of the Doppler spectrum of the received signal (see e.g.: Brown, 1972; Brown and Clifford, 1973; Thomson and Coulter, 1974).

Most acdar systems are either monostatic, that is the same antenna is used for both transmitting and receiving, or "short-baseline" bistatic in which the transmitter and receiver are separated by, at most, only a few hundred meters. With these systems it is now possible to monitor more-or-less continuously the altitude of many structural features and the vector velocity at selected levels. The systems are not suited, however, for measurements of the vertical temperature profile.

The technique described in this paper for determining temperature gradients of surface-based and elevated inversions within the planetary boundary layer requires a monostatic sounder estimating the height of the inversion base and a "long-baseline" bistatic sounder for measuring the characteristics of refracted signals. The refracted signals are measured at distances ranging from about 3 to 15 km.

In a windless atmosphere, refraction arrivals will return to the ground only if temperature at some level exceeds the surface value. Fortunately, because the analysis of refraction measurements is so greatly complicated by wind, the surface and elevated inversions, which we are measuring because of their effect on the dispersion of pollutants, occur most frequently during calm or light wind conditions. The nocturnal surface (or slightly elevated) inversions are strongest in large high pressure weather systems in which clear skies enable the surface to efficiently cool by radiation. When light winds are present, they frequently are of the "drainage" type and, thus, dependent upon local terrain conditions. In many areas the lowermost elevations are enveloped in ground fog.

Several previous studies have discussed the "ducting" of sound in low level inversions (Ingard, 1953; Weiner and Keast, 1959; Kriebel, 1971; and Lyon, 1973). Chung (1972) studied wind and temperature variations in the boundary layer using infra-sonic, bistatic techniques.

II. Model for Ray Paths in the Lower Troposphere

We assume a two or three layer model for the planetary boundary layer which is analogous to those frequently employed for studies of propagating gravity waves (Müller, 1969; Stilke and Müller, 1972, Stilke, 1973). Below

the inversion layer the upward temperature is assumed to be small and negative, within the inversion the gradient is positive and relatively large and in the atmosphere above it is again negative. From the surface to a height H_1 , the temperature gradient T_1' is negative and less than the adiabatic (Figure 1). Within the inversion layer T_2' is positive and may be as much as $20^\circ/\text{km}$. Above the inversion layer ($z > H_2$) the temperature gradient T_2' is again negative and its magnitude less than T_1' . If the inversion is a surface inversion, $H_1 = 0$. But in urban environments the inversion may be somewhat elevated during the same conditions in which inversions are surface based in rural areas (Panofsky, 1969).

Ray paths for waves refracted in an inversion layer are also shown in Figure 1. A zone of silence extends from the source to the arrival distance of ray B. In the vicinity of the closest arrival at the "caustic" distance, R_c , the sound level is high due to refractive focusing. Individual rays arriving beyond the caustic do have different arrival angles and phases. Thus, they may either constructively or destructively interfere. When the incidence angle on an inversion exceeds a certain critical angle, such as for ray E, rays will no longer be sufficiently refracted to return to the surface.

Ray paths and travel times for the two or three layer models were computed using the standard method for constant velocity gradient profiles (see e.g.; Officer, 1958). The slight nonlinearity in the sound speed profile for a constant temperature gradient was neglected. For the nearly horizontal rays with which we were concerned, the formulation given by Chung (1972) would also have been suitable. Chung's method is useful when significant horizontal wind is present. For this the effective sound speed

profile is defined by

$$C_e(z) = C(z) + V_x(z) - V_x(0)$$

where C is the sound speed, V_x the component of the wind along the transmitter-receiver line and z is height.

III. Methods for Estimating the Vertical Temperature Profile

In order to determine the atmospheric parameters T_1' , T_2' and H_1 , we assume first that the height H_1 of the base of the transition layer may be determined using a vertically pointing monostatic radar. The caustic is located using either a mobile receiver or in a permanent installation using an array of receivers spaced at 500 m to 1 km intervals stretching outward from the transmitter. Either the boundary of the so called zone-of-silence or the characteristics of the high intensity zone may be used to identify R_c . Some sound may be present in the zone-of-silence due to scattering (Weiner and Keast, 1959) but its level is, normally, very low. If possible it is also advantageous to measure the signal travel time, t_c , from the source to a receiver located near the caustic.

The values of T_1' and T_2' may be estimated from H_1 , R_c and t_c . Let $\hat{t}(R)$ be the reduced travel time

$$\hat{t}(R) = t(R) - \frac{R}{C_0}$$

where C_0 is the sound speed at the surface

and R is the source to receiver distance.

Figure 2 shows $\hat{t}$ versus R for various combinations of T_1' and T_2' with $H_1 = 200$ m. Figure 3 illustrates an interpretation diagram based on $\hat{t}_c$

the reduced travel time at the caustic, and R_c . To use the diagram the measured values are plotted with R_c and $\hat{t}_c$ as abscissa and ordinate, respectively. Then T_1' and T_2' can be interpolated from the plotted curves. As an example, a measurement of $R_c = 12$ km, $\hat{t}_c = 40$ msec is shown. Temperature gradients of $-1.5^\circ/\text{km}$ and $14^\circ/\text{km}$ are, thus, estimated for below and within the inversion layer. To assess the error, $\delta T_2'$, of T_2' we write

$$\delta T_2' \approx \frac{\partial T_2'}{\partial H_1} \delta H_1 + \frac{\partial T_2'}{\partial R_c} \delta R_c + \frac{\partial T_2'}{\partial \hat{t}_c} \delta \hat{t}_c$$

where δH_1 , δR_c and $\delta \hat{t}_c$ are the errors in the measured values. To obtain typical numerical values consider an atmosphere with $T_1' = -3$ deg/km, $T_2' = 10$ deg/km and $H_1 = 200$ m. For this atmosphere $\frac{\partial T_2'}{\partial H_1} = .04$ deg/km/m, $\frac{\partial T_2'}{\partial R_c} = 1 \cdot \text{deg/km}^2$ and $\frac{\partial T_2'}{\partial \hat{t}_c} = .04$ deg/km/sec.

To demonstrate the measurement accuracies which these values imply, assume an experiment in which only one of the measured parameters H_1 , R_c , or $\hat{t}_c$ is in error. If a resultant error of 1 deg/km in T_2' is acceptable, it requires that if H_1 is the parameter in error, that its error be $\delta H < 25$ m; if R_c is in error that $\delta R_c < 1$ km; or if $\hat{t}_c$ is in error, that $\delta \hat{t}_c < 25$ msec.

Monostatic acdar measurements may be used to locate layer boundaries to within ranging errors of less than about 25 m. Thus, a satisfactory estimate of H_1 is not a problem. The error in R_c depends upon the distance between measuring stations.

The determination of $\hat{t}_c$ is more difficult. Measurements we have taken (Figure 4) indicate that the error in estimating arrival time is on the order of 10 msec. This is sufficiently precise. However, the total travel

time for a distance of 10 km is only about 30 sec. Thus an error in $\hat{t}_c$ of even 25 msec is approximately only .1% of the travel time. In fact, the limiting factor in determining $\hat{t}_c$ is probably not the signal to noise ratio but rather inhomogeneities in the horizontal temperature field. We do have, however, aircraft observations which indicate that the maximum standard deviation of $\hat{t}_c$ variations due to horizontal temperature variations will in many cases be less than 5-10 msec.

Fortunately, an estimate of T_2' can be made without using $\hat{t}_c$. Figure 5 shows R_c plotted versus T_2' for three values of T_1' . From the figure it is apparent that if the curve for $T_1' = -3$ deg/km is used to make the interpretation based on the measured value of R_c , the error in T_2' will be on the order of .5 deg/km if $0 > T_1' > -.6$ deg/km. In Figure 6 a second diagram for making this estimate of T_2' is presented. This diagram may be used for any values of T_2' and H_1 .

Travel time measurements may also be used to estimate the temperature gradient, T' , for a ground-based inversion layer. In this case signals are received at all distances. Figure 7 illustrates the reduced travel time versus distance curves for a surface-based inversion.

IV. Techniques for Field Measurements

Refraction observations made to date have been obtained using a bistatic system operating at 200 Hz over distances ranging from about 1.5 to 10 km.

The transmitter consists of a 200 Hz CW source, and a variable tone burst generator which drives a series of power amplifiers. In order to be able to experiment with variable antenna beamwidths, a "phased array" transmitter configuration was chosen. Four 60 watt (CW) power amplifiers

drive four separate woofer enclosures, each with nine 8" woofers. The separation of the approximately 1 m³ enclosures may be varied to adjust the acoustic beamwidth from essentially that of an isotropic source to one of only a few degrees beamwidth. Measurements of transmitted acoustic power ($\approx$ 12 watts) show the emitted patterns to be in agreement with theory at least to within the experimental error resulting from ground reflections.

The mobile receiving unit is van mounted. Because a directional antenna at 200 Hz cannot be made readily portable, an "isotropic" sensitive microphone is used as the antenna-receiver. The received signal is pre-amplified, filtered in an active bandpass filter (CF = 200 Hz, BW = 10 Hz) and both the filtered and unfiltered outputs recorded on a multi-channel analog tape recorder. The filtered signal is also envelope detected, averaged on an integrating RMS voltmeter and then displayed as "signal strength" on a strip chart recorder.

Figure 4 is an example of typical unfiltered and filtered received signals obtained during one experiment during fall of 1973. Experiments to date have focused on examining the signal behavior as a function of time of day at different ranges. Fluctuations in signal strength, fading, appear to be strongly dependent on the inversion dynamics. Periodic variations which could be associated with propagating gravity waves are evident and the signal scintillation markedly increases as radiative heating breaks up the nocturnal inversion. Whenever inversions are present, the signal to noise ratio does appear to be adequate for temperature profile estimates.

Field measurements during summer of 1974 will include acoustic measurements of the caustic distance and travel time, aircraft or digital sonde measurements of the vertical temperature and wind profiles, and electronic micro-microbarograph recordings of atmospheric gravity waves.

ACKNOWLEDGEMENTS

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FIGURE CAPTIONS

1. Model temperature profile and refraction ray paths.
2. Reduced travel time versus distance for $H_1 = 200$ m. The numbers under each curve give T_2' in deg C/km.
3. Interpretation diagram to find T_1' and T_2' . $H_1 = 200$ m.
4. Unfiltered and filtered received signal output, showing signal onset. Range was 3-6 km.
5. Caustic distance versus T_2' .
6. Interpretation diagram for determining T_2' computed for $T_1' = -3^\circ$ C/km, but useful for full range of T_1' values. Dashed line example shows an interpretation of $T_2' = 15^\circ$ C/km for measured $R_C = 15$ km and $H_1 = 300$ m.
7. Reduced travel time versus range for ground based inversion layer.

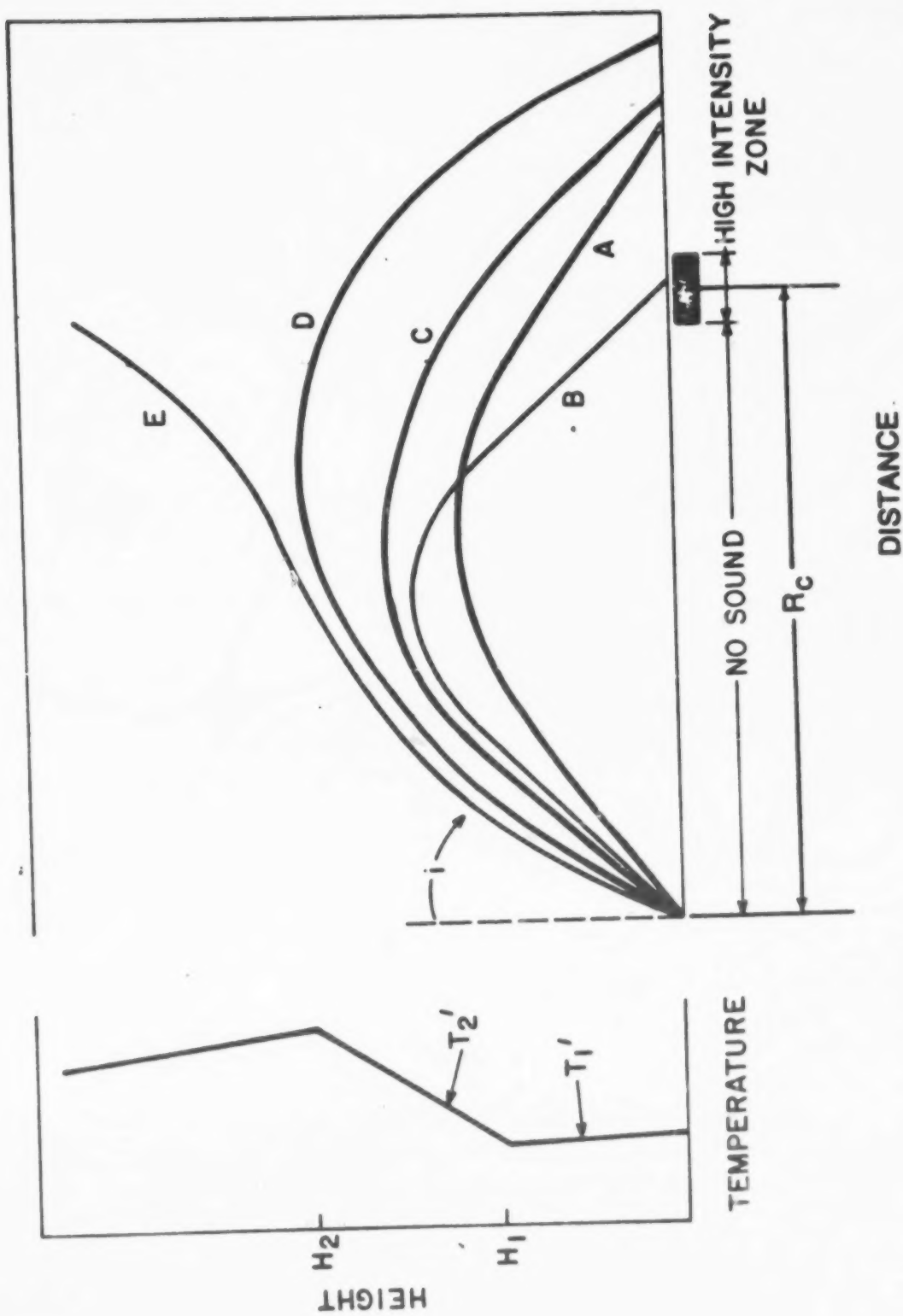


FIGURE 1

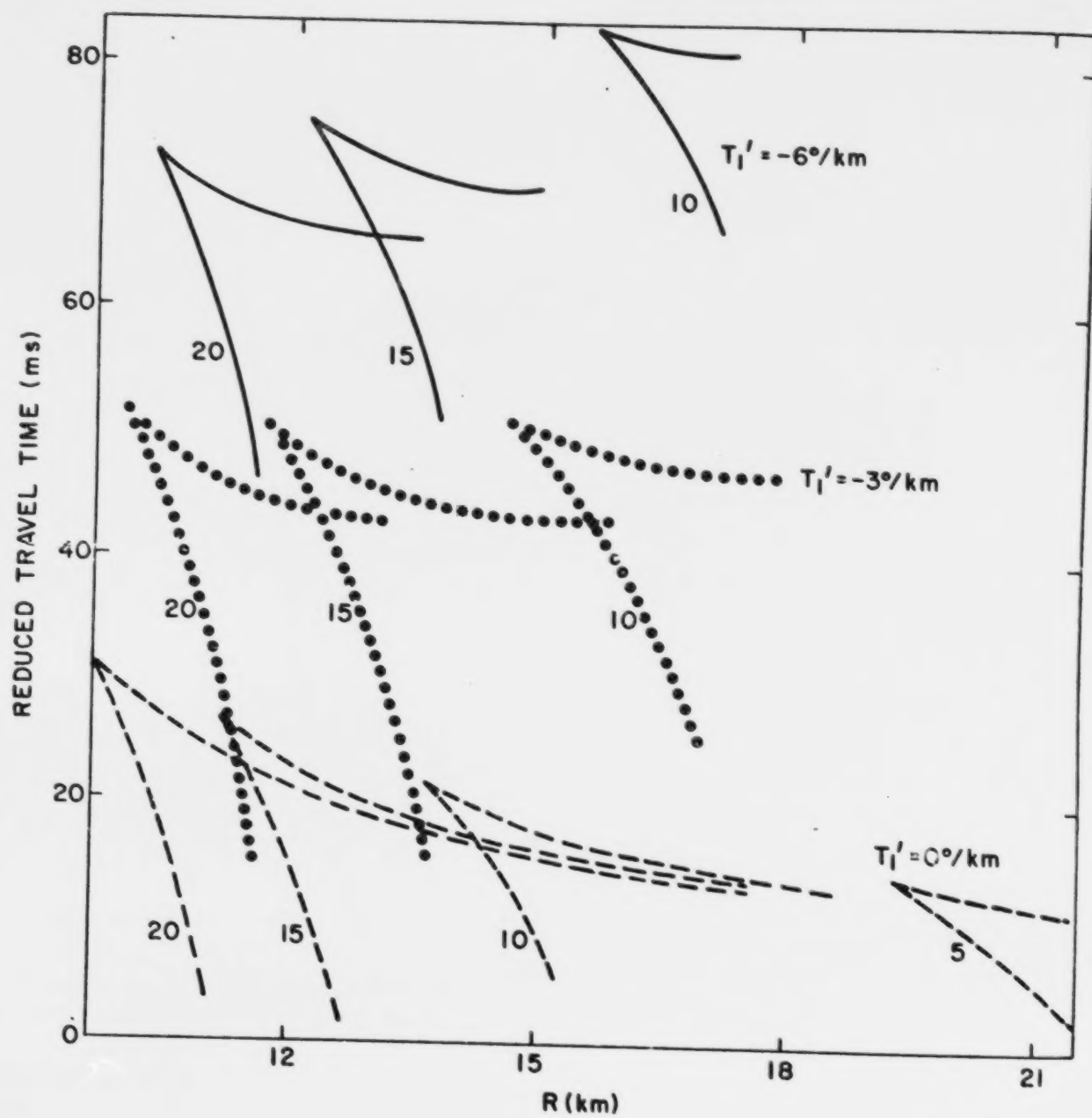


FIGURE 2

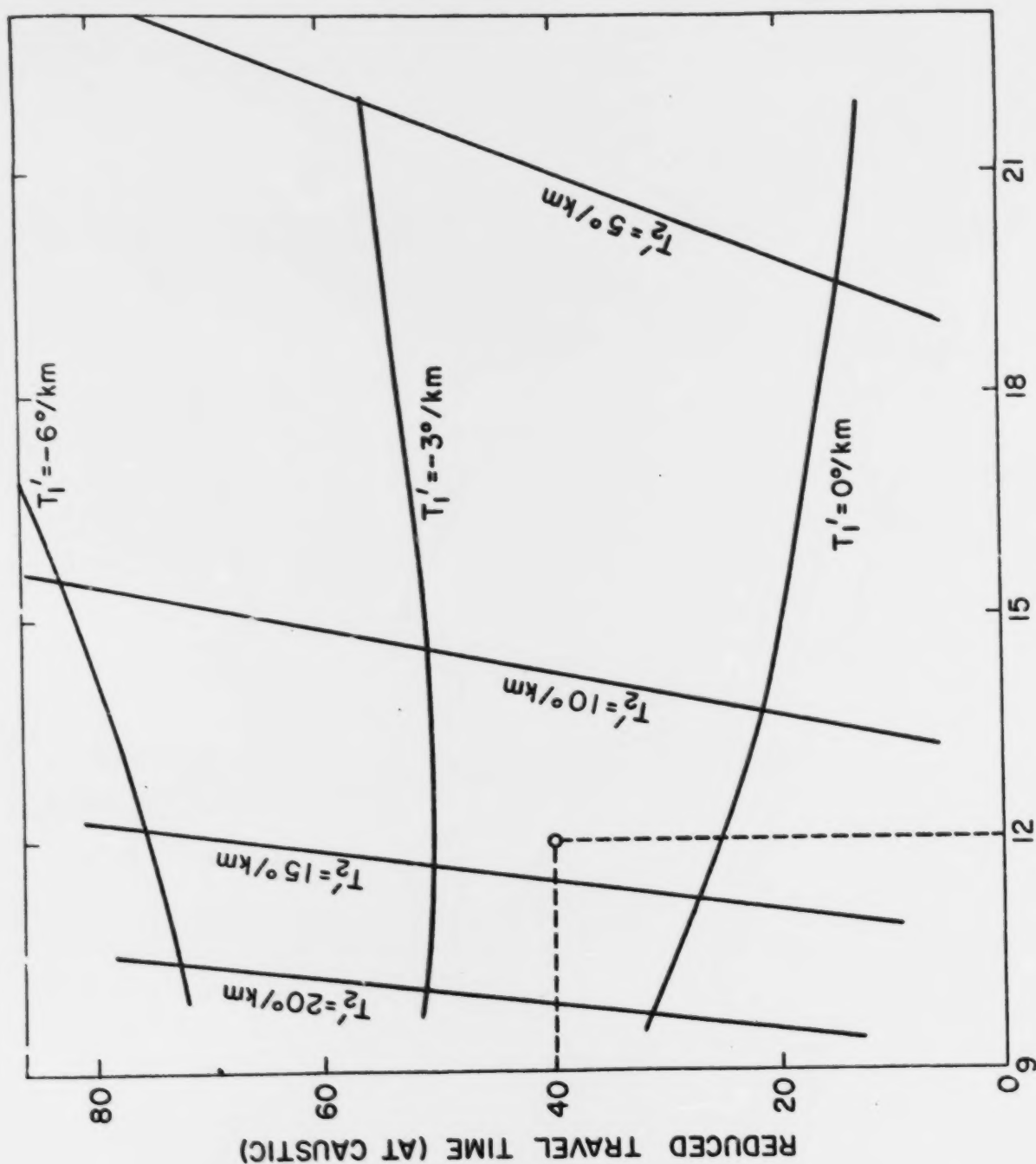
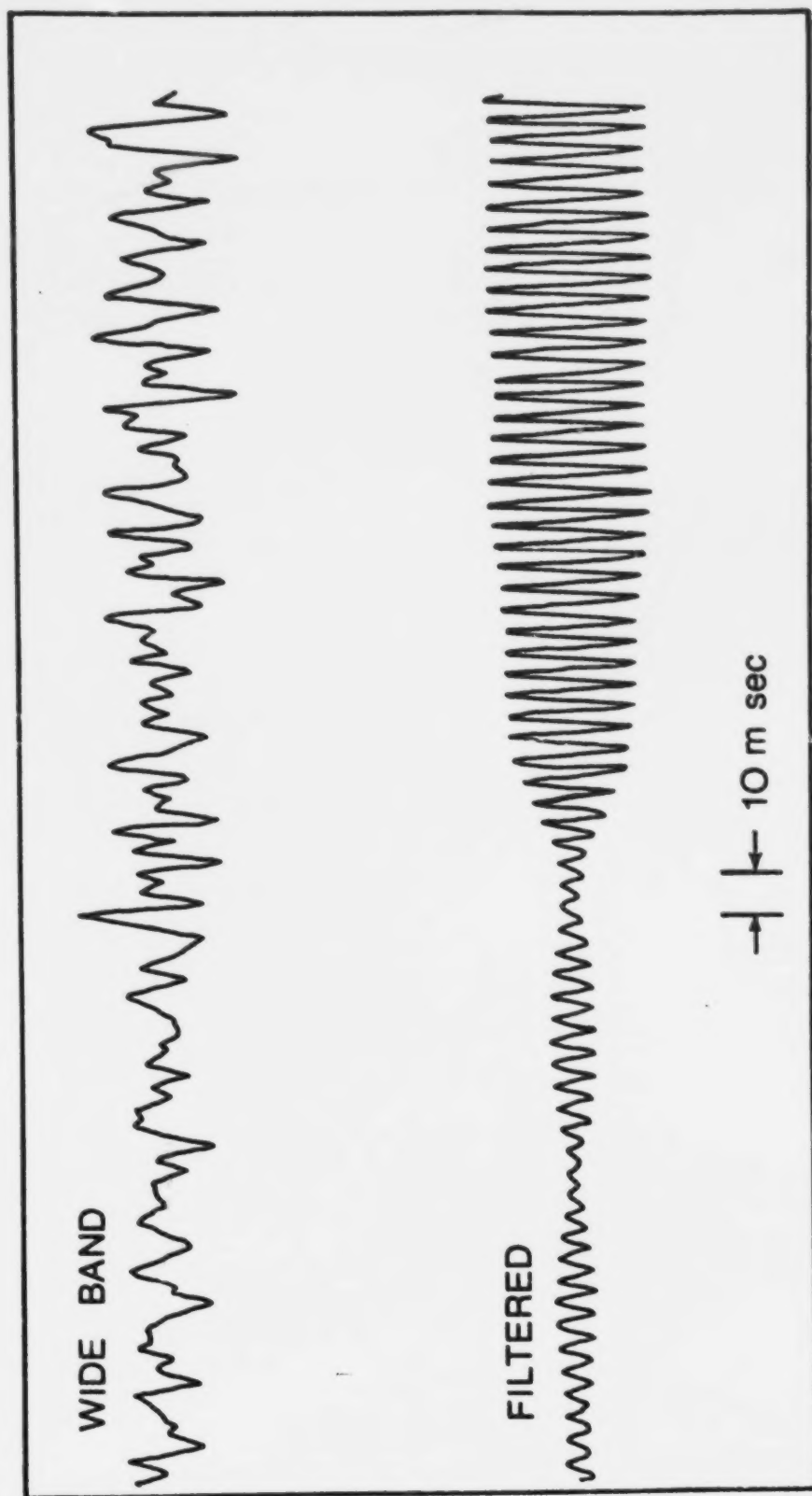


FIGURE 3
CAUSTIC DISTANCE (km)



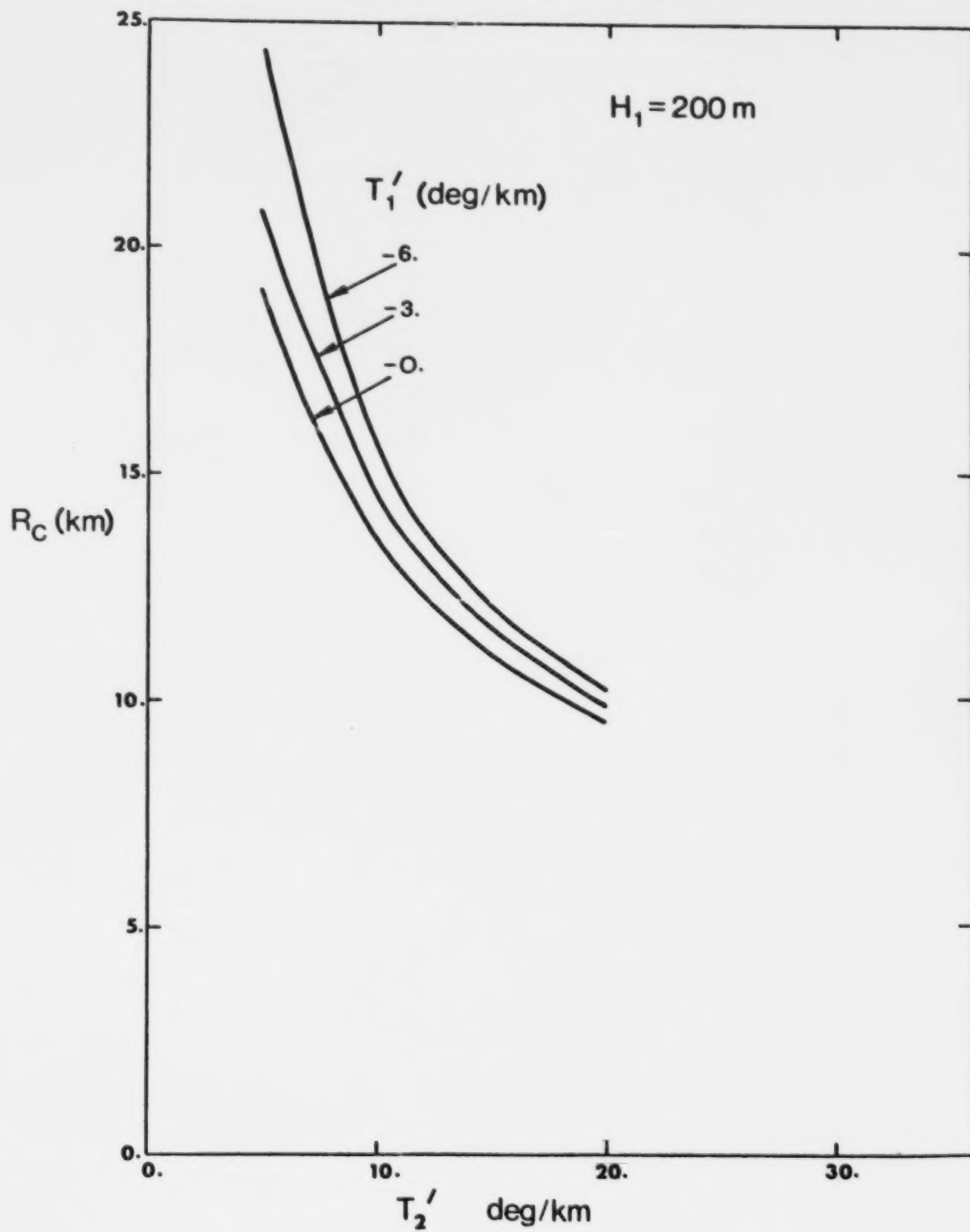


FIGURE 5

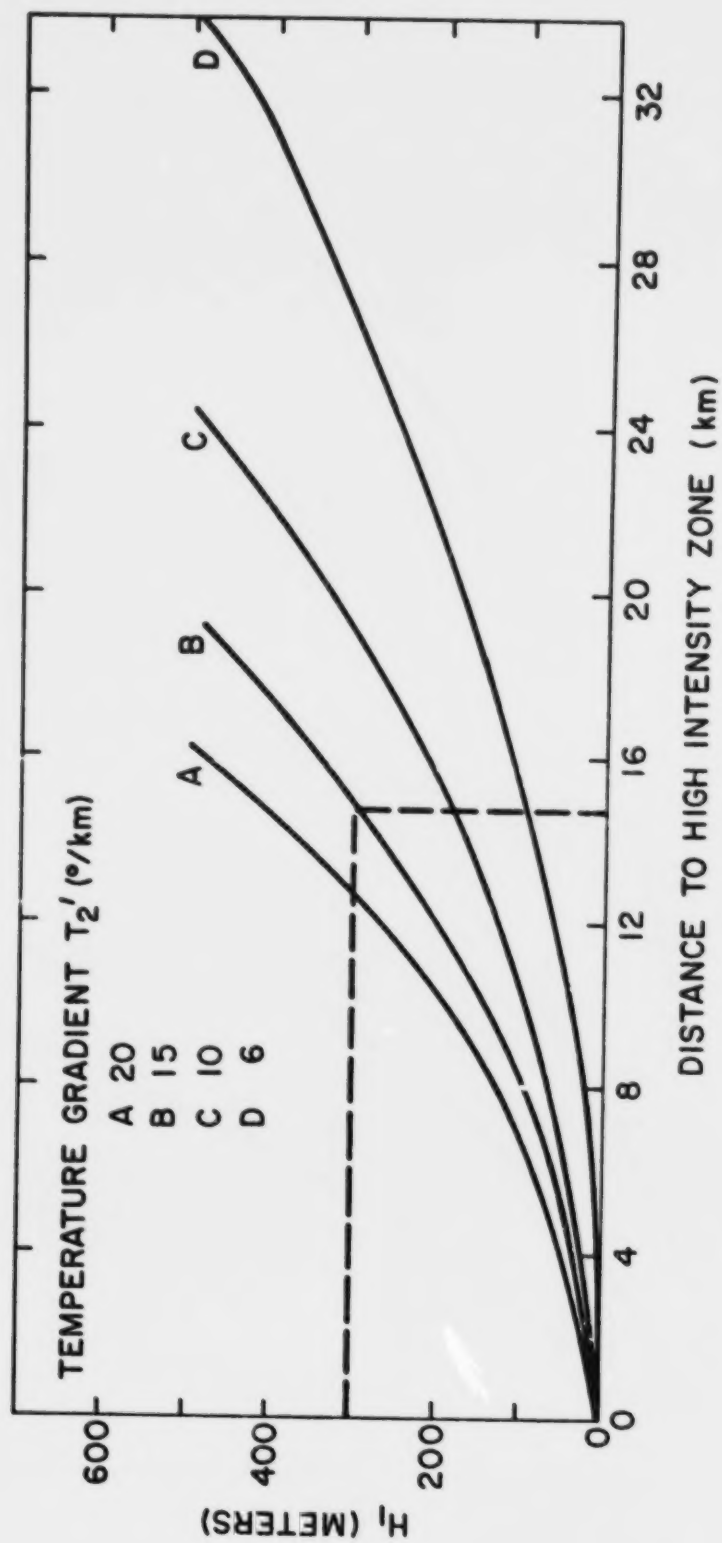


FIGURE 6

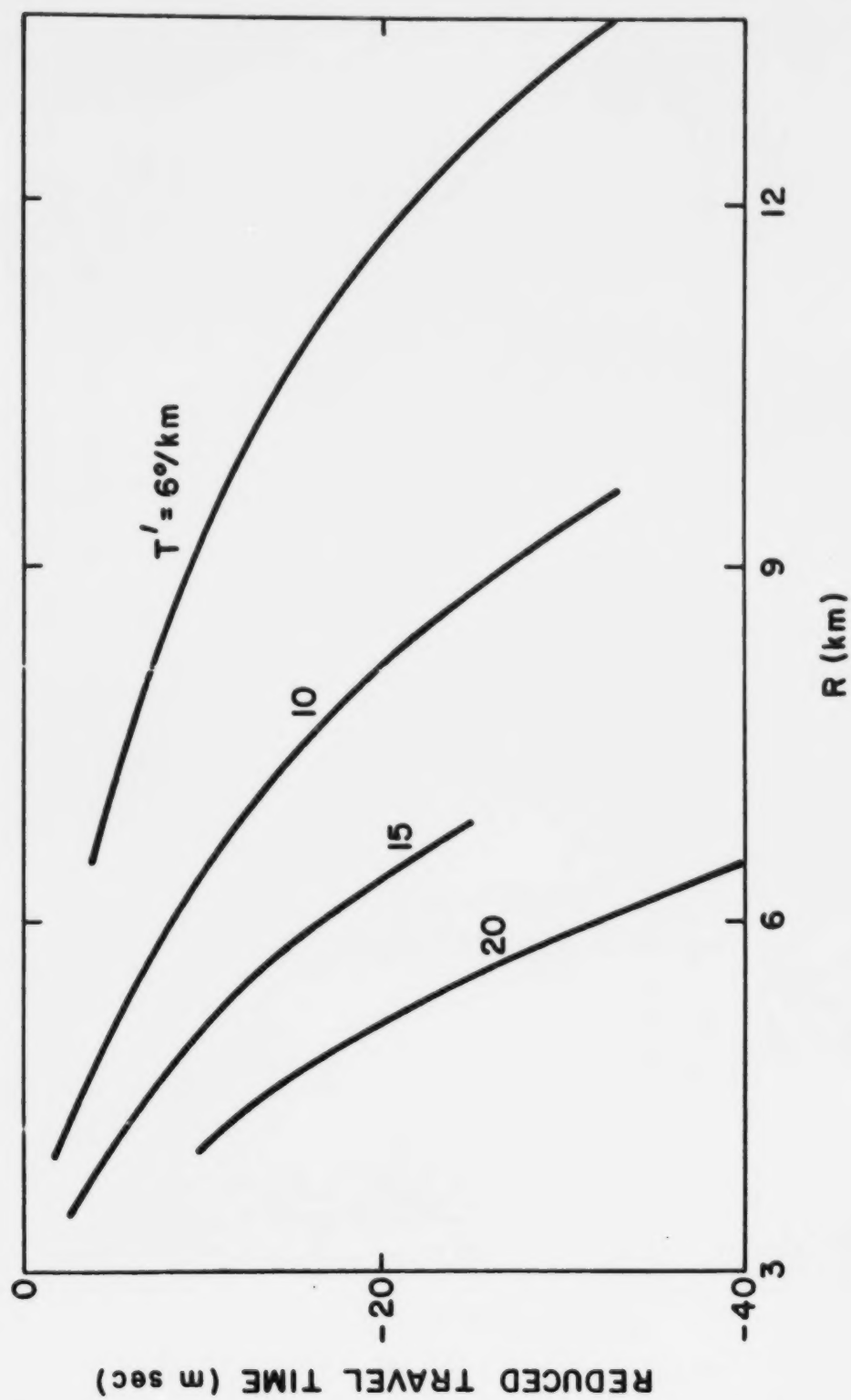


FIGURE 7

6.0 ANALYSIS AND SIMULATION OF PHASE-COHERENT
ACDAR SOUNDING MEASUREMENTS

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3790 Instruments and techniques
ANALYSIS AND SIMULATION OF PHASE-COHERENT ACDAR
SOUNDING MEASUREMENTS

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The phase-surface geometry and its dependence upon system and atmospheric parameters for both monostatic and bistatic acdar sounders is discussed. The observed Doppler frequency shift is shown to be a consequence of the motion with respect to the equiphase surfaces of many distributed atmospheric scatterers. Because acdar measured average Doppler frequencies and Doppler spectra are integral functions of system-related and atmospheric structure-dependent weighting functions, application of simple models which assume signal scattering only along the antenna beam axis may result in significant wind velocity measurement errors. It is further shown that accurate quantitative estimates of C_T^2 and C_V^2 for thin turbulent layers require detailed analysis of the bistatic acdar common volume. Two techniques, based on distributed scatterers and random phasors, respectively, are used for simulating acdar signal phase and amplitude fluctuations.

Abstract

The phase-surface geometry and its dependence upon system and atmospheric parameters for both monostatic and bistatic acdar sounders is discussed. The observed Doppler frequency shift is shown to be a consequence of the motion with respect to the equiphase surfaces of many distributed atmospheric scatterers. Because acdar measured average Doppler frequencies and Doppler spectra are integral functions of system-related and atmospheric structure-dependent weighting functions, application of simple models which assume signal scattering only along the antenna beam axis may result in significant wind velocity measurement errors. It is further shown that accurate quantitative estimates of C_T^2 and C_V^2 for thin turbulent layers require detailed analysis of the bistatic acdar common volume. Two techniques, based on distributed scatterers and random phasors, respectively, are used for simulating acdar signal phase and amplitude fluctuations.

I. Introduction

If the Doppler frequency shift measured with a phase-coherent acdar system resulted from signal scattering by a single point target, the observed Doppler shift would depend only upon the acdar operating frequency, the transmitter-receiver separation, the vector velocity of the scatterer and the line integral of the transmitter-scatterer-receiver acoustic ray path. In general, however, the received signal is the resultant or sum of many components. Although the acoustic scattering may be relatively more efficient within a given layer or region smaller than the volume defined by the combined transmit and receive antenna beams, individual moving point scatterers, such as raindrops in a cloud, are randomly distributed in space. Thus, the received signal from which one can derive a Doppler spectrum and an average Doppler frequency, represents an integral space-time average. The Doppler spectrum will depend not only upon the system frequency and geometry but also upon the antenna beam-width(s) and the distribution of energy within the transmitter beam. The atmospheric variables which influence the shape of the Doppler spectrum include the mean vertical temperature and vector wind profiles, the 3-dimensional turbulent velocity and temperature fields and, finally, the angular dependence of the scattering coefficients of all the individual scatterers which contribute to the total received signal.

Acdar Doppler measurements have been used to study thermal plume velocities (Beran et al., 1971a; Beran et al., 1971b), winds in the planetary boundary layer (Beran and Willmarth, 1971; Beran and Clifford, 1972; Mahoney et al., 1973), gravity waves (Hooke et al., 1973; Beran et al., 1973), and boundary layer turbulence (Bean et al., 1973).

Interpretation of Doppler shifted signals has, with few exceptions, been based on the work published by Clifford and Brown (1970), Beran and Clifford (1972), Brown (1972), Brown and Clifford (1973) and Georges and Clifford (1972). In the above papers the nature of acoustic propagation through a refracting and turbulent atmospheric medium to the scattering volume was discussed. Thus, both changes in the magnitude of the Doppler shift as a consequence of changes in the wave vector along the propagation path and at the scatterer were assessed, and broadening of the Doppler spectrum due to propagation through a turbulent atmosphere has been evaluated. One result of the modeling work discussed in this paper is an analysis of the Doppler shift and spectrum produced by many discrete scatterers distributed and moving in space.

When one is attempting to quantitatively analyze the relative importance of both system and atmospheric parameters upon the nature of the received signal, it is useful to be able to conduct experiments using a "controlled" rather than the real, and somewhat capricious, atmosphere. Thus, we've chosen, initially, to numerically model or "simulate" using several different techniques, the time-dependent, phase and amplitude fluctuations of a complex radar signal. The modeling results will be directly compared with radar Doppler measurements (and airborne meteorological measurements) once the phase-coherent sounder presently under construction at Penn State is completed.

II. Phase Space Geometry and Signal Doppler Shifts

The Doppler frequency shift of a received acoustic signal may be associated with the translation of a "scatterer" through equiphase surfaces, the family of surfaces of constant path length, defined by the transmitter-receiver system operating at a wave length λ . The Doppler shift, f_d , may be written as the rate of change of phase, ϕ ,

$$f_d = - \frac{d\phi}{dt} = - \frac{1}{\lambda} \frac{dL}{dt} = - \frac{1}{\lambda} \vec{V} \cdot \nabla L \quad (1)$$

where L is the ray path length from the transmitter to the receiver which passes through the scatterer moving at velocity $\vec{V}$. An equivalent expression in terms of the wave vectors $\vec{K}_0$ of the transmitted wave and $\vec{K}_s$ of the scattered wave is

$$f_d = \frac{1}{2\pi} (\vec{K}_s - \vec{K}_0) \cdot \vec{V} \quad (2)$$

Both expressions illustrate the dependence of the Doppler frequency shift on the motion of a scatterer relative to the surfaces of equal phase.

The simplest equiphase surface geometry is associated with a monostatic sounder operating in a non-turbulent, isothermal atmosphere with no horizontal or vertical motions. For this case the equiphase surfaces are spherical shells separated by 2π radians in phase or $\Delta r = \lambda$ in space. Because the Doppler frequency is proportional to the rate at which a moving scatterer "cuts" through the equiphase surfaces, radial velocities such as vertical at the zenith or horizontal in the up and downwind directions at the horizon will produce the maximum observed Doppler frequencies. Clearly, the phase space geometry is independent of the antennas which serve only as illumination "weighting" functions. In fact, for the above case, the

acdar geometry is analogous to Doppler radar and may be analyzed using the same principles. (See e.g. Lhermitte, 1966; Browning and Atlas, 1966; and Browning and Wexler, 1968).

Consider the trajectory of a single scatterer moving horizontally with the mean wind and passing above an acdar. The relationship between accumulated signal phase and distance may be written

$$\Delta\phi = \phi_n - \phi_{n-1} = 2\pi : \Delta r = r_n - r_{n-1} = \lambda \quad (3)$$

where r_n and r_{n-1} are adjacent equiphase surfaces (figure 1). The horizontal distance required for a moving scatterer at height z to create a phase path length change of 2π is:

$$\Delta x = (r^2 - z^2)^{1/2} - ((r - \lambda)^2 - z^2)^{1/2} \quad (4)$$

The Doppler frequency at any given displacement and height is minus the local derivative of the plotted $d\phi/dx$ curve (figure 2) times the scatterer velocity:

$$f_d = - \frac{d\phi}{dt} = - \frac{d\phi}{dx} \cdot \frac{dx}{dt} = - \frac{d\phi}{dx} \cdot v_H \quad (5)$$

The phase space geometry of a bistatic acdar is somewhat more complicated because separation of the transmitter and receiver creates a position-dependent separation of the equiphase surfaces. In terms of an x, y, z coordinate system in which the origin is located at the midpoint of the chord (x axis) between the receiver and transmitter, which are situated at $+d$ and $-d$, respectively, and y and z are in the cross chord and vertical directions,

$$L = [(d+x)^2 + y^2 + z^2]^{1/2} + [(d-x)^2 + y^2 + z^2]^{1/2} \quad (6)$$

For a bistatic system operating in an isothermal, windless atmosphere, the equiphase surfaces are, thus, ellipsoids of revolution. The transmitter-receiver separation is $D = 2d$. The single scatterer Doppler frequency is

$$f_d = -\frac{2}{\lambda} \left[u \frac{\partial \ell}{\partial x} + v \frac{\partial \ell}{\partial y} + w \frac{\partial \ell}{\partial z} \right]$$

where $\ell = L/2$ and $V = \hat{i}u + \hat{j}v + \hat{k}w$, or

$$f_d = -\frac{4}{\lambda L} \frac{ux(1 - 4d^2/L^2) + vy + wz}{1 - 16 \frac{x^2 d^2}{L^4}} \quad (7)$$

In the midpath, $x = 0$, plane

$$f_d = -\frac{4}{\lambda L} (vy + wz) \quad (8)$$

In the case of a monostatic acdar, horizontal motions at the zenith did not produce Doppler shifts. But for a bistatic system both vertical and "crosspath" motions at midpath can produce Doppler shifts. Clearly, the complete expression (7), which includes u , v and w components must be used for analyzing Doppler data obtained with bistatic systems which include one vertically pointing and one tilted antenna. Note, that the observed Doppler shift not only depends upon the inverse of the wavelength but also upon the transmitter-receiver separation and the position of the scatterer.

Equation 7 may be used to determine the family of $d\phi/dx$ curves, as for the monostatic case in figure 2, for any given bistatic acdar system. The Doppler shift associated with a scatterer moving at any point in space is then obtained by scaling by the appropriate velocity, $\vec{V}$.

Two orthogonal, say N-S and E-W oriented, bistatic systems simultaneously sounding the same region may be used to determine both the horizontal and vertical velocity components. If each system has narrow beam antennas which are pointed along its x axis, $y = 0$ and the observed Doppler frequency, from (8), will be the result of vertical velocities only.

$$f_d = - \frac{4}{\lambda_d} (w z)$$

If the antennas from the two systems are then synchronously pointed away from their respective x axes, $y > 0$ and the observed Doppler shifts will be proportional to the E-W and N-S wind components. The Doppler shift from vertical motions is the same for both systems and may be extracted.

System N-S

$$f_{d_{NS}} = - \frac{4}{\lambda_d} (V_{EW} y + w z)$$

System E-W

(9)

$$f_{d_{EW}} = - \frac{4}{\lambda_d} (V_{NS} y + w z)$$

In the normal atmosphere vertical temperature and wind gradients refractively distort the "ideal" equiphase surfaces. Temperatures decreasing (increasing) with height tend to flatten (peak) the equiphase surfaces. The vector wind changing with height creates significant asymmetries in the phase space which locally alter $d\phi/dx$, $d\phi/dy$ and $d\phi/dz$. The extent to which observations must be corrected for refractive effects depends upon the particular atmospheric conditions at the time of the experiments (Georges and Clifford, 1972). In our numerical simulation studies, ray

tracing has been used to compute the actual phase space geometry for each specified situation.

III. System and Atmospheric Weighting Functions

A primary objective of many acdar research programs is to quantify the relationships of the acoustic extinction and volume backscatter coefficients, $\alpha(r)$ and $\beta(r)$, with the meteorological variables C_T^2 , C_V^2 , and the state parameters and winds. In this section we show that quantitative estimates of $\alpha(r)$ and $\beta(r)$ require, especially for bistatic systems, careful analysis of the "system" function.

A received acdar signal is not a "point-target" echo but rather the resultant signal from many scatterers of varying phase and amplitude distributed throughout the volume defined by the antennas and the pulse length in space. In order to evaluate the received power as a function of range we write the "acdar" equation:

$$P(r) = P_o \frac{A_c}{A_T} \cdot \frac{A_r}{R^2} L_v \cdot e^{-\int_{\text{Trans.}}^{\text{Scat.}} \alpha(r) dr} \cdot \beta(\theta, r) \cdot e^{-\int_{\text{Scat.}}^{\text{Rec.}} \alpha(r) dr} \quad (10)$$

where P_o = peak transmitted power

A_c = area common to transmitter and receiver beams

A_T = area of transmit antenna

A_r = area of receiver antenna

R = range from scatterer to receiver

r = range along L

L_v = length of scattering volume in space

$\alpha(r)$ = extinction coefficient

$\beta(\theta, r)$ = scattering angle dependent volume scatter coefficient

All parameters other than $\alpha(r)$ and $\beta(r)$ are dependent upon the system.

Hence, we designate

$$S(r) = \frac{A_c}{A_T} \cdot \frac{A_r}{R^2} L_v \quad (11)$$

the system function.

For monostatic systems¹ the system function is easily evaluated since $A_c = A_T$. Thus $S(r)$ is simply proportional to $A_r/R^2 \cdot L_v$. However, for the bistatic geometry in which the transmitter and receiver are separated and one beam is tilted with respect to the other, determination of the scattering volume as a function of range can be a difficult analytical problem. The volume defined by the transmitter and receiver antennas and the pulse length in space is $V(r) = A_c(t, \text{ or } r) \cdot L_v$ (figure 3). But the scattered wave front returned to the receiver at time t is tilted $\phi/2$ with respect to both the transmitter and receiver axes.¹ Because the equitime wave front is tilted at $\phi/2$, the length of the scattering volume L_v changes from $v_s \tau/2$, as for the monostatic case, to $v_s \tau/2 \cos \phi$.

Since the value of A_c varies continuously as a function of range, and varies significantly even along the length of the scattering volume L_v , $V(r)$ can best be evaluated as

$$V(r) = \int_{r_o}^{r_o + L_v} A_c(r) dr \quad (12)$$

For the bistatic case A_c is the area common to two ellipses (figure 4), each the resultant of cutting an antenna (transmit and receive) cone at an angle of $\phi/2$. The ellipses have major axes

¹Note that the equitime surfaces are coincident, as expected, with the equi-phase surfaces.

$$\tilde{b} = \frac{R \sin \beta}{\cos(\phi/2 + \beta)} \quad , \text{ transmit}$$

and

$$b = \frac{R' \sin \alpha}{\cos(\phi/2 - \alpha)} \quad , \text{ receive}$$

(13)

where R and R' are as indicated in figure 4. Each can be geometrically related to r . With $\tilde{b}$ and b defined, the value of A_c is determined to be

$$A_c = ab \cos^{-1} \left(\frac{x_1}{b} \right) + \tilde{a}\tilde{b} \cos^{-1} \left(\frac{y_1}{\tilde{b}} \right) - |y_1 \xi| \quad (14)$$

where x_1, y_1 are the intersections of the ellipses shown in figure 4, $a, \tilde{a}$ are the semi-major axes, and ξ is the distance between the centers of the ellipses. All are known functions, albeit quite complicated, of α, β, ϕ, D and r . Equation 14 may be numerically integrated to yield $V(r)$ to any required accuracy.

Figure 5 illustrates the results of performing the integration to evaluate the common volume as a function of range. As a pulse of width $v_p \tau$ traverses the common volume the resulting signal from $V(r)$ typically varies as shown in figure 5. Between points x_1 and x_2 (figure 3) the volume (and, subsequently, signal level) increases rapidly through 3 orders of magnitude in a matter of 200 msec. Between points x_2 and x_3 , when the sensed volume is completely within both beams $V(r)$ increases much less rapidly. In fact, for ~ 500 msec it increases simply as r^2 . Finally, from $x_3 \rightarrow x_4$ the volume falls off rapidly, though not so rapidly (≈ 500 msec) as it rose between x_1 and x_2 . The lengths of these segments is a strong function of ϕ, α, β and D , but are easily evaluated geometrically. The shape of these curves is independent of τ (unless $v_p \tau \gg x_2 - x_1$), even though the volume sensed is, of course, directly related. Also, if $\alpha = \beta$, i.e. the transmitter and

receiver are of equal beamwidth, then for most cases $x_2 \approx x_3$ and the middle portion of the curves disappears.

Including the rest of the system function $(\frac{A_r}{r^2 A_T})$ results in curves such as figure 6. These curves indicate the variation of the signal strength, assuming uniform scattering throughout, as a pulse traverses the common volume. There is a strong dependence on α , β , ϕ , D and the strength varies considerably as the volume is traversed. There is a rapid rise from x_1 to x_2 followed by a decrease ($\propto \frac{1}{r^2}$) from x_2 to x_3 , because $\frac{1}{r^2} \frac{1}{A_r} \rightarrow \frac{1}{r^4}$, and then from x_3 to x_4 it falls off very rapidly.

The implications of this are readily seen. Assume, for example, a thin layer of scatterers of thickness much less than $x_4 - x_1$. In this case the value of C_V^2 and/or C_T^2 determined can vary by a large amount depending upon the location of the layer within the common volume. On the other hand, if the layer is thick and encompasses a large portion of the common volume, then even with a constant scatter coefficient the signal will vary considerably as a function of range. In the section from $x_2 - x_3$, one might be able to compensate for the $\frac{1}{r^2}$ drop-off by analog multiplication by r^2 . Unfortunately, this is not possible in the lower and uppermost regions of the common volume. Proper compensation can, however, be readily handled digitally, just by specifying α , β , ϕ and D .

The Doppler spectrum which results from the many scatterers that contribute to the resultant received signal depends upon not only system but also atmospheric parameters. We write the Doppler spectrum $S(f)$ as

$$S(f) df = G(\alpha, \phi) W(\phi) d\alpha \quad (15)$$

where $G(\alpha, \phi)$ is related to the distribution of energy within the antenna beams and the antenna pointing angle, and $W(\phi)$ is the scattering angle dependent volume scatter coefficient, $B(\theta, r)$, expressed in terms of the antenna pointing angle. For an individual scatterer, f and the antenna pointing angle may be related using (7). However, in order to determine the average Doppler shift of a "many scatterer" signal, the Doppler spectrum must be evaluated. One technique is that employed by Bello (1965) in which the average frequency is given by

$$\bar{f} = \int f S(f) df / \int S(f) df \quad (16)$$

Application and numerical evaluation of this integral (Section V) clearly demonstrates the dependence of the derived Doppler frequency upon both the system parameters and the ambient atmospheric conditions.

IV. Models for Signal Simulation

We are using several different modeling techniques to simulate signal phase and amplitude fluctuations from scatterers distributed in space. The first, designated DS, is a "distributed scatterer" model in which the signal as a function of time is derived from artificial scatterers moving in a specified (temperature and wind profile) atmosphere and illuminated by the transmit-receive antennas. In a second "RP" model, the individual signal contributions are simply simulated using a set of phasors of random phase, amplitude and angular velocity. The distribution of phasor amplitudes and angular velocities is proscribed as the basis of system and atmospheric parameters. However, no assumptions are made regarding the actual atmospheric conditions and the actual acoustic signal scattering.

In the DS model, which is two-dimensional, all significant signal scattering is forced to occur within a layer of limited vertical extent. The scatterers are assumed to represent small regions (or "eddies") of enhanced scatter or "partial-reflection". In a 3-dimensional geometry, the scatterers would be flat "platelets" with no vertical dimension, in the two-dimensional model they are short lines parallel to the surface.

The existence and horizontal position of each scatterer is determined using a "flip of a coin" technique. Thus, in the horizontal the scatterers are uniformly, randomly distributed. In order to generate a layer of finite vertical thickness, the uniform random numbers generated to produce the horizontal distribution are transformed, two at a time, into any array of normally distributed random numbers using:

$$N_1 = (-2 \ln RN_1)^{1/2} \cos(2\pi RN_1)$$

$$N_{1+1} = (-2 \ln RN_1)^{1/2} \sin(2\pi RN_1)$$

where

N_1, N_{i+1} = normally distributed random numbers

and

RN_1, RN_{i+1} = uniformly distributed random numbers.

The normally distributed random numbers have a zero mean and unity variance and in this form are not suitable for use as spatial coordinates. Thus, they are modified using:

$$z_1 = \sigma N_1 + \bar{z}$$

$$z_{i+1} = \sigma N_{i+1} + \bar{z}$$

with z_1 and z_{i+1} representing the vertical coordinates of scatterer 1 and $i+1$. The total thickness in meters of the scattering layer, situated at mean height $\bar{z}$, is approximately 2σ .

Using a ray tracing technique, the horizontal coordinate and angle of rays propagated from the transmitter are determined at a level 2σ below $\bar{z}$. Thus, in the DS model refractive temperature effects are included although, at least to date, asymmetric distortion of the phase space by wind has not. From the base of the layer individual rays are then propagated into it. In order to ensure that scatterers which exist within the layer are intersected, the mean spacing between rays is constrained to be less than the mean horizontal scatterer dimension. When a ray intersects a scatterer, its phase angle and amplitude are stored in an array from which the resultant signal phase and amplitude are calculated.

For the results presented in this paper, the signal amplitude $[G(\alpha, \phi) \cdot W(\phi)]$ associated with a single scatterer was assumed to be a function of the position of the scatterer in the antenna beam and the angle of incidence of the ray upon the "flat" scatterer. The energy in the transmitter beam $G(\alpha, \phi)$, was assumed to be Gaussian distributed about the beam axis and the atmospheric scattering "angular dependence", $W(\phi)$ to be dependent on the cosine of the incidence angle. Figure 7 illustrates several combined amplitude weighting functions for different antenna angles. Maximum signal is clearly associated with scatterers located at the zenith in the boresight of vertically pointing antennas. A major objective of planned field experiments at Penn State is evaluation of $W(\phi)$ as a function of planetary boundary layer structure.

The resultant signal at any given time is thus the vector sum of all the individual scatterer in-phase and quadrature phase components

$$\begin{aligned} A_r &= \sum_{i=1}^n A_{r1} \\ A_q &= \sum_{i=1}^n A_{q1} \end{aligned} \tag{17}$$

where n equals the total number of intercepted scatterers.

In order to simulate motion of the scatterers within the layer, the array of scatterers is incrementally shifted a horizontal distance (less than the mean width of the scatterers) and the new set of ray-scatterer interceptions and the resultant A_r and A_q computed. Clearly, a Doppler shift represents, in effect, a continuously increasing (or decreasing) apparent phase path length. Because the phase always lies between 0 and 2π and yet tends to accumulate in one direction, it is necessary to both

determine the direction of rotation of the resultant phasor and to remove the "2 π ambiguity." In the DS model, this was accomplished by computing the average phase change for the entire scatterer array -- assuming that the average phase change could be associated with motion of the centroid of intercepted scatterers. The direction of rotation of the resultant phasor was thus defined in terms of the change in path length to the centroid. It was found that by allowing scatterer shifts of the order of one-half the scatterer size, that average phasor rotations of no more than 2 π radians between adjacent time steps occurred.

The "RP" model uses as its basis any number of phasors. Although each phasor represents an individual scatterer, no assumptions are made regarding the nature or structure of the scatterers which the phasors represent. Each phasor rotates at a different rate, has a different initial phase angle and, finally, a different amplitude. The rotation rate corresponds to the scatterer's Doppler frequency. Initially, phase angles are randomly distributed. At later times they are determined by the movement of the scatterers relative to the phase space. Thus, here the basic information is $\frac{d\phi}{dt}$ from each scatterer, whereas in the DS model it is ϕ .

The received signal, however, consists only of the time-varying amplitude and phase of the resultant phasor. As in the DS model the resultant is the vector sum of all the individual phasor contributions, i.e.,

$$A_r(t) = ((\sum_1 A_1 \cos(\omega_1 t + \phi_1))^2 + (\sum_1 A_1 \sin(\omega_1 t + \phi_1))^2)^{1/2}$$

$$\phi_r(t) = \tan^{-1} \frac{\sum_1 A_1 \sin(\omega_1 t + \phi_1)}{\sum_1 A_1 \cos(\omega_1 t + \phi_1)}$$

where

$$E_r(t) = A_r(t)e^{j(\omega_r(t)t + \phi_r(t))}$$

$A_r, \sum A_i \cos(\omega_i t + \phi_i)$, is the in-phase and $A_q, \sum A_i \sin(\omega_i t + \phi_i)$, the quadrature phase component of the received signal. By measuring $\frac{\Delta\phi_r}{\Delta t}$ as a function of time one obtains both the Doppler frequency and the amplitude as a function of time. The resultant Doppler spectrum can, thus, be obtained.

The input spectrum is a function of the system parameters and atmospheric conditions. The amplitude spectrum is determined by the antenna weighting functions, the distance to the scatterers and the specified scattering angle dependence. The frequency spectrum is determined by the phase space geometry and the wind velocity components.

For any model such as this, which requires finite difference techniques, it must be assumed that the scatterer exists for a length of time long compared to the time step of the model. Furthermore, it is necessary to assume an effective scatterer "center" in order to determine the phase. In actuality, scatterers probably occupy some finite volume.

V. Characteristics of Simulated Signals

The DS model was first tested by performing a "beam-filling" experiment. Consider a vertically pointing monostatic "CW" radar operating in an isothermal, windless (except at the scattering layer) atmosphere. Assume, initially, its beam to be devoid of scatterers. If a patch of randomly distributed scatterers (as described in the previous section) moves into the beam, initially only up-Doppler scatterers on the upwind edge of the beam will be illuminated. Thus, although the instantaneous Doppler frequency may significantly depart from the mean, the tendency will be for the path length to continuously decrease (figure 8) and for the average received frequency to exceed the transmitted. After the antenna beam is filled to the zenith point, both up and down Doppler scatterers will contribute to the received signal, and after the entire beam is filled, the average phase path length change will be zero. At any given time the instantaneous slope of the phase versus time plot may correspond to any one of the many Doppler frequencies present in the spectrum of the received signal.

Next the DS model was used to examine the differences between Doppler frequency shifts predicted on the basis of single scatter theory and those produced by distributed scatterers in a layer contained within the antenna beam (or in the case of a bistatic system, within the common volume).

A tabulation of the average Doppler frequency, $\overline{\Delta\phi/\Delta t}$ as a function of antenna pointing angle, ϕ , for a single scatterer on the beam axis and a many scatterer layer at two heights, 123 and 246 m, is presented and plotted in Table 1 and figure 9, respectively. In order to approximate a "worst" case condition of beam spreading in a highly turbulent mixing layer, the simulation was based on a super-adiabatic temperature gradient of $-2^\circ\text{C}/100\text{ m}$ and a very large beamwidth of 18° .

Note the decrease in average Doppler frequency which results from the combined weighting function acting on the distributed scatterers. Due to the heavier weighting of scatterers positioned closer to the zenith, the peak of the Doppler spectrum is shifted to a lower frequency. Note also that two scattering layers moving at the same velocity, but at different heights will produce different Doppler frequencies. In terms of the phase space geometry, the result is simply the consequence of a scatterer (at the same horizontal displacement from the zenith) at a lower level intercepting more phase surfaces per unit time than one at a higher level. The results suggest that a properly analyzed Doppler spread may provide a measure of vertical wind shear.

Figures 10 and 11 illustrate typical signal phase and amplitude fluctuations obtained using the DS model. The dependence of the average Doppler frequency and the signal amplitude fading upon the antenna pointing angle is evident.

The above results regarding the differences between single and arrays of scatterers have also been noted in the analysis of phase-coherent troposcatter radio signals (Birkemeier et al. (1968); Atlas et al. (1969); and Birkemeier and Thomson (1968)). Changes in the Doppler spectrum are, clearly, most significant when systems with large antenna beamwidths are used to probe layers with highly directional scattering or "reflecting" characteristics. If the acoustic scattering only weakly depends upon the scattering angle and an acdar system has narrow antenna beams, a simple model, equations (1) or (2), may be used to satisfactorily derive wind velocities from the calculated Doppler spectrum.

Examples of the random phasor "RP" model output are shown in figures 12, 13 and 14. Rather than the accumulated phase, its time derivative is directly computed. With this model as opposed to the DS model, it is not necessary to make assumptions regarding changes in position of the scattering centroid or to average phase data from several time steps to derive the "instantaneous" Doppler shift.

For the example shown, the amplitudes of individual phasors were specified to be Gaussian distributed about the mean. That is

$$A_1 = A_0 \exp [- (\omega_1 - \bar{\omega})^2 / 2\sigma_\omega] \quad .$$

Such a distribution could be associated with the signal received from a thermal rising within the beam of a vertically pointing radar. In the model $\bar{\omega}\Delta t = \text{const.} = 0.07$. Thus, if $\bar{\omega} = 5$ Hz, a single time step corresponds to 14 msec.

The illustrated output was produced using only 15 phasors. As shown by Slack (1946), the probability density of n phasors is not Rayleigh distributed when n is less than about 10. Prior to using the RP model for predicting signal phase behavior, the statistical properties of signal amplitude fluctuations computed for varying numbers of phasors were compared with and verified against Slack's results. The purpose was to be able to adequately simulate the signal's properties using as few independent phasors (scatterers) as possible.

Figure 12 is representative of simulated signal amplitude fluctuations. As expected, minimum amplitudes tend to occur when the Doppler frequencies (figure 13) are either a minimum or a maximum. In other words, when the

relatively large amplitude phasors which control the "average" Doppler shift interfere to "0," the smaller phasors associated with scatterers at the edge of the antenna beam, will tend to control the signal phase fluctuations.

Figure 14 illustrates both the input spectrum (inset) of the 15 phasors and the resultant power spectrum of $d\phi/dt$. Because the resultant phase of a number of rotating phasors may "instantaneously" shift by $n\pi$ ($n \geq 1$) radians, the resultant spectrum will normally be wider than the input. When the resultant Doppler frequencies are numerically simulated, the maximum and minimum frequencies are $\pi/\Delta t$ and $-\pi/\Delta t$, respectively. This effect is also easily seen on figure 13.

The simple RP model results shown here have not included variable rotation rates and phase angles for each phasor at each time step. Thus, the signal is repetitive at $t = 2\pi/\Delta f$ where Δf is the smallest frequency difference between any two phasors. When variable rotation rates and phase angles are included, which does more correctly simulate the motion of scatterers within the phase space, apparent periodicities in the signal phase and amplitude fluctuations disappear. However, the basic shape of the Doppler spectrum is not altered.

The primary advantage of the RP model is that few (≥ 15) phasors are required to numerically simulate the received signal and derive a suitable estimate of its Doppler spectrum. Our computational costs for running the "small n " RP model were a small fraction of those of runs of the "several hundred n " DS model. If, however, a measured acdar signal is clearly non-Rayleigh, an RP model may be used to relate the signal amplitude and phase fluctuations to observed structural features.

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Table I Doppler Frequency (rad/sec) as a Function of Antenna Pointing Angle and Layer Height.

Elevation	Pointing Angle, ϕ ($^{\circ}$)					
	0.0	4.5	9.0	13.5	18.0	22.5
Single Scatter						
z = 123	0.00	1.26	2.68	4.28	6.31	9.11
Multiple Scatter						
z = 123	0.00			3.07	5.16	7.99
z = 246	0.00	0.43	1.19		3.86	

FIGURE LEGEND

- Figure 1. Two-dimensional equiphase surfaces in an isothermal, windless atmosphere.
- Figure 2. Accumulated signal phase versus scatterer displacement for a single scatterer moving horizontally through the beam of a vertically pointing sounder.
- Figure 3. Cross section of bistatic link antenna and pulse geometry.
- Figure 4. Intersection of transmit and receive antenna beams on a surface of equitime or equiphase.
- Figure 5. Common volume as a function of range for pulse lengths of 40, 80, 120 and 240 ms. $\alpha = 1^\circ$, $\beta = 2^\circ$, $D = 100$ m, $\phi = 10^\circ$.
- Figure 6. System function as a function of range and transmitter-receiver separation. Pulse lengths are 40 and 100 ms, $\alpha = 1^\circ$, $\beta = 2^\circ$, and $\phi = 20^\circ$.
- Figure 7. Combined amplitude weighting functions for antenna pointing angles range from 0 to 9° from zenith and cosine dependent scattering angle dependence. Antenna beamwidth = 9° .
- Figure 8. Accumulated total phase from scatterers moving into a vertically pointing beam. $f_d = \overline{\Delta\phi/\Delta t}$.
- Figure 9. Comparison of mean Doppler frequencies computed for multiply scattering layers of 246 and 123 m, and for a single scatterer at 123 m and varying distances from the zenith.
- Figure 10. Example of accumulated phase versus time output of DS model.

Figure 11. Example of signal amplitude versus time output of DS model.

Figure 12. Amplitude returns from "RP" model versus time, with t subdivisions every $4\Delta t$, where Δt is determined from $\bar{\omega}\Delta t = .07$.

Figure 13. Doppler frequencies returns from "RP" model versus time.

Figure 14. Received power spectrum of $\frac{d\phi}{dt}$ and input power spectrum. Units of $\frac{d\phi}{dt}$ the same as for ω_i .

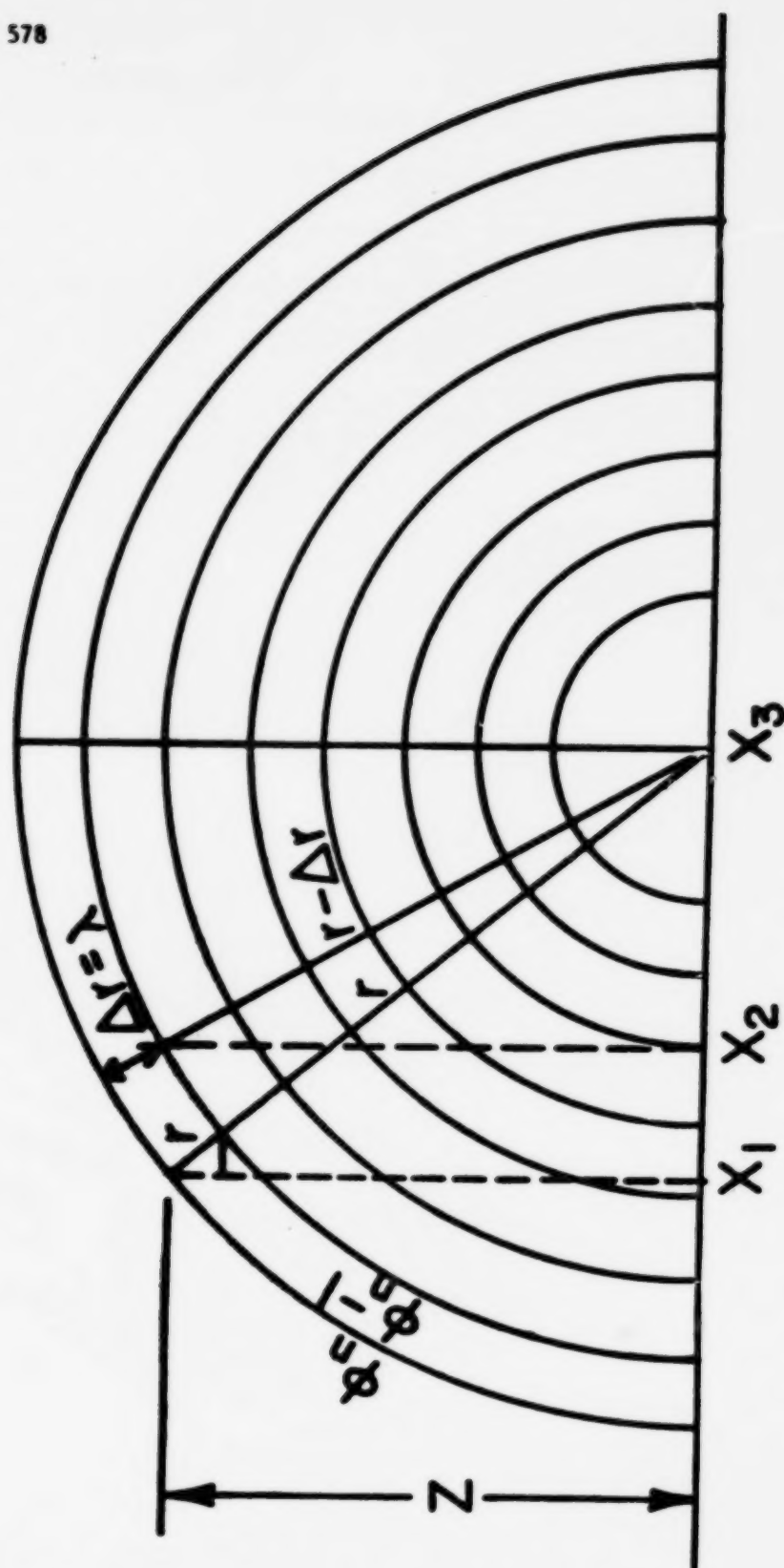


FIGURE 1

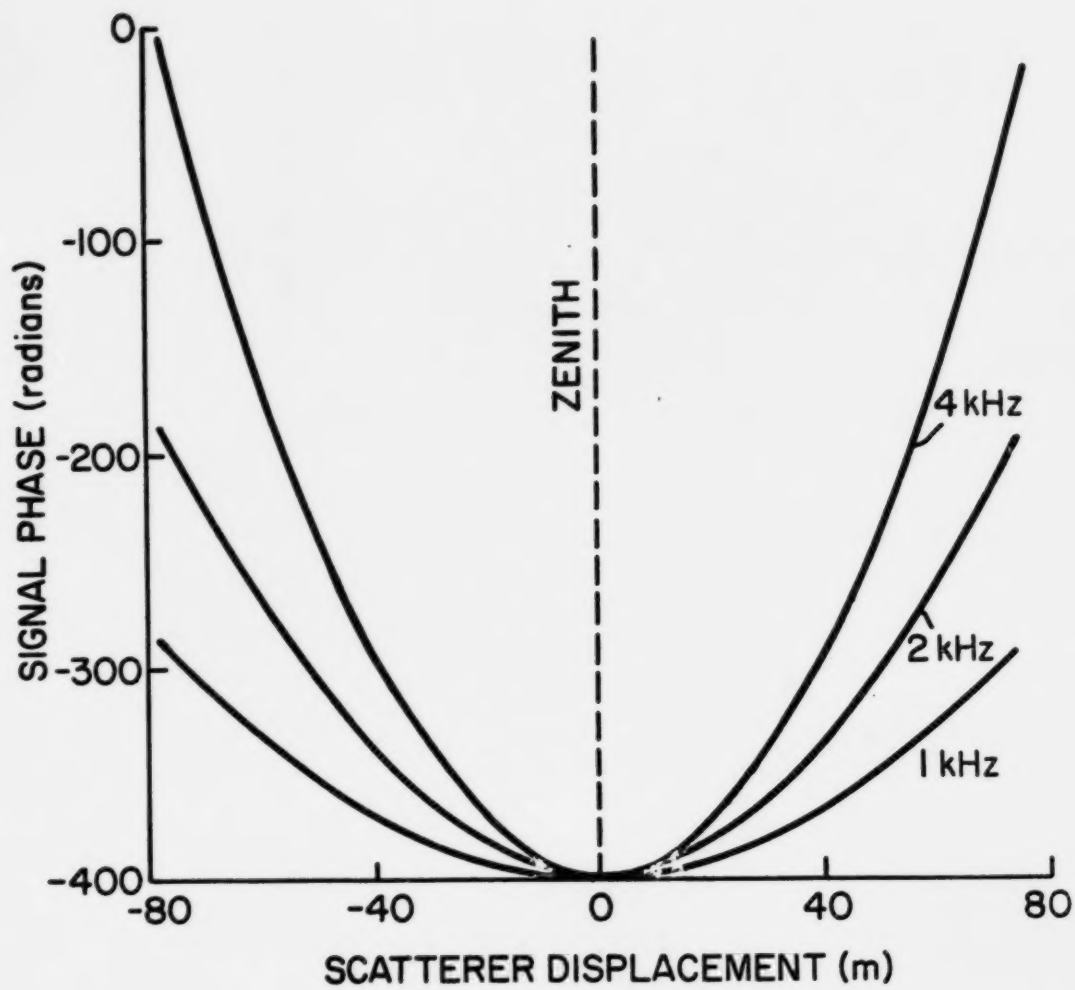


FIGURE 2

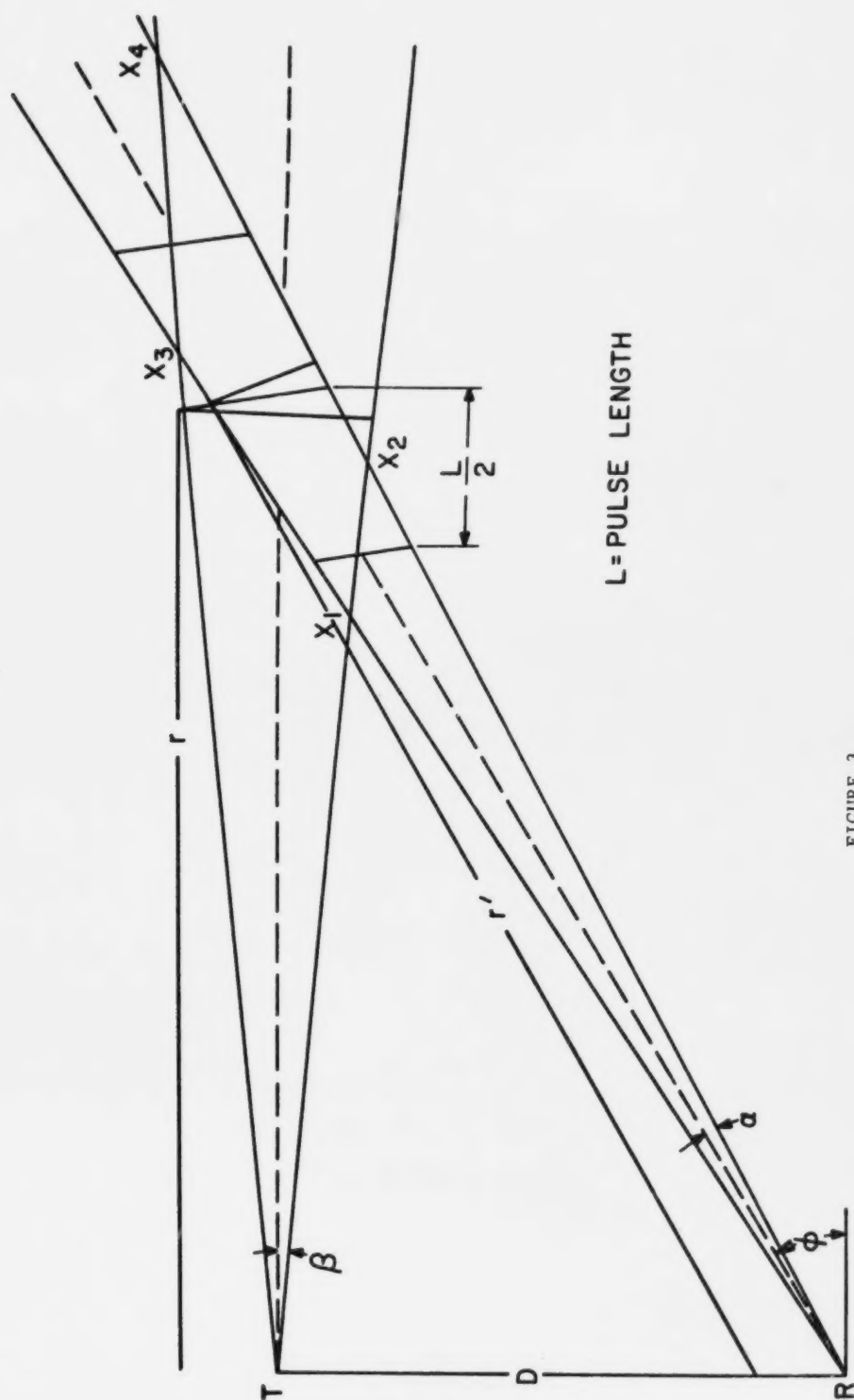


FIGURE 3

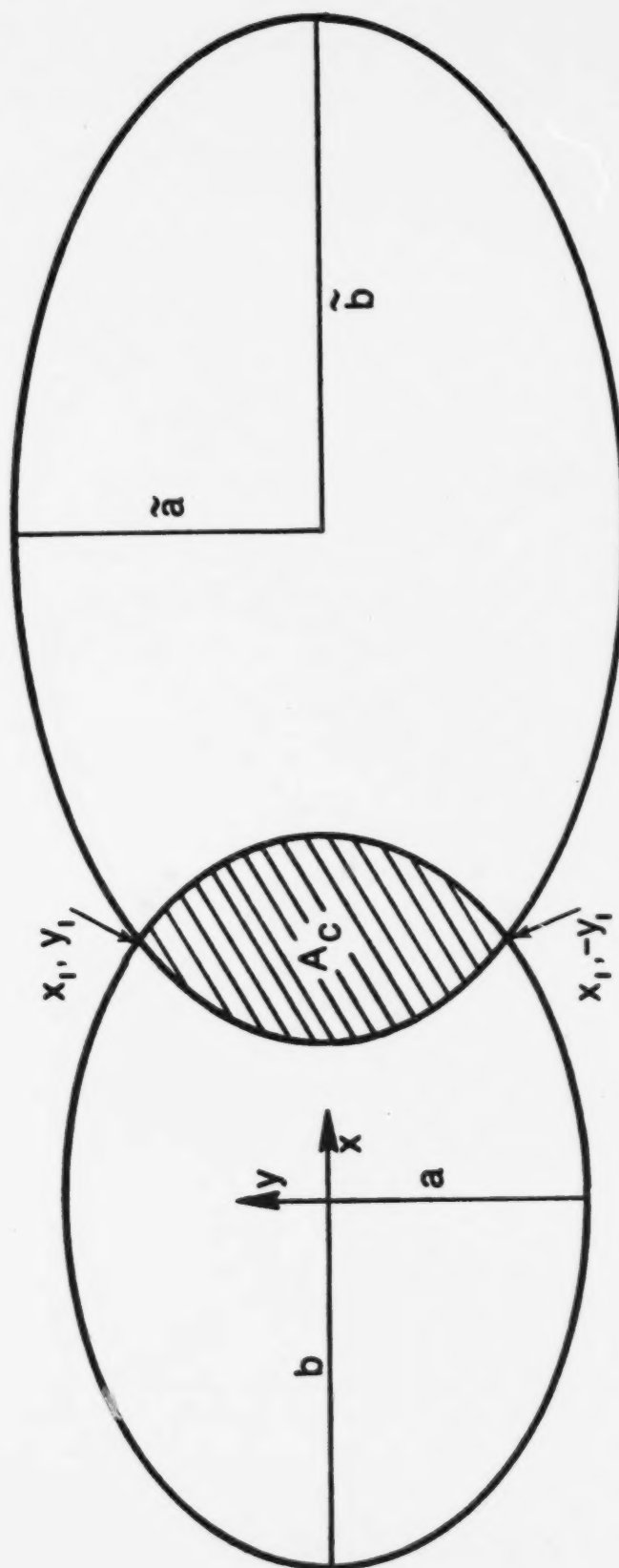


FIGURE 4

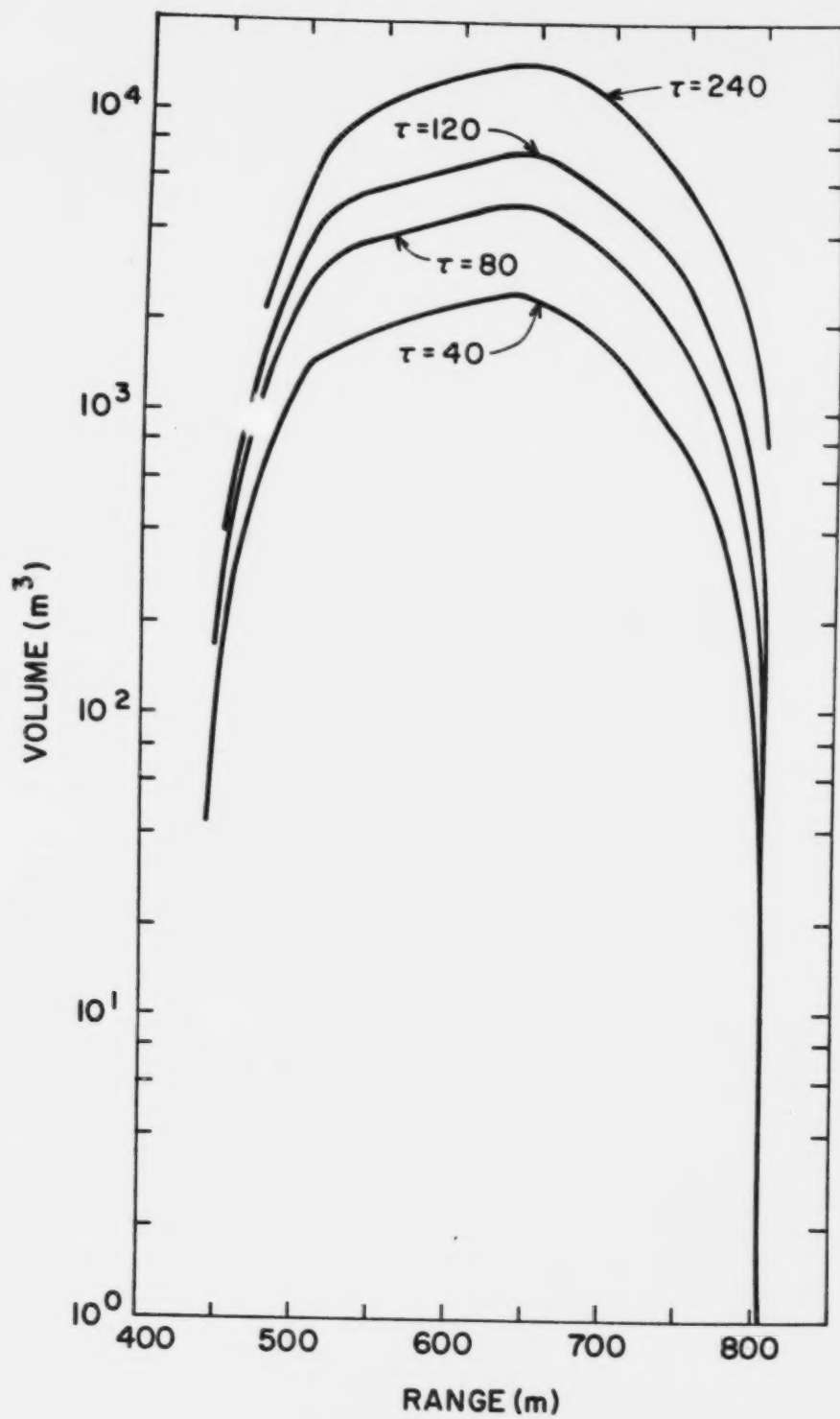


FIGURE 5

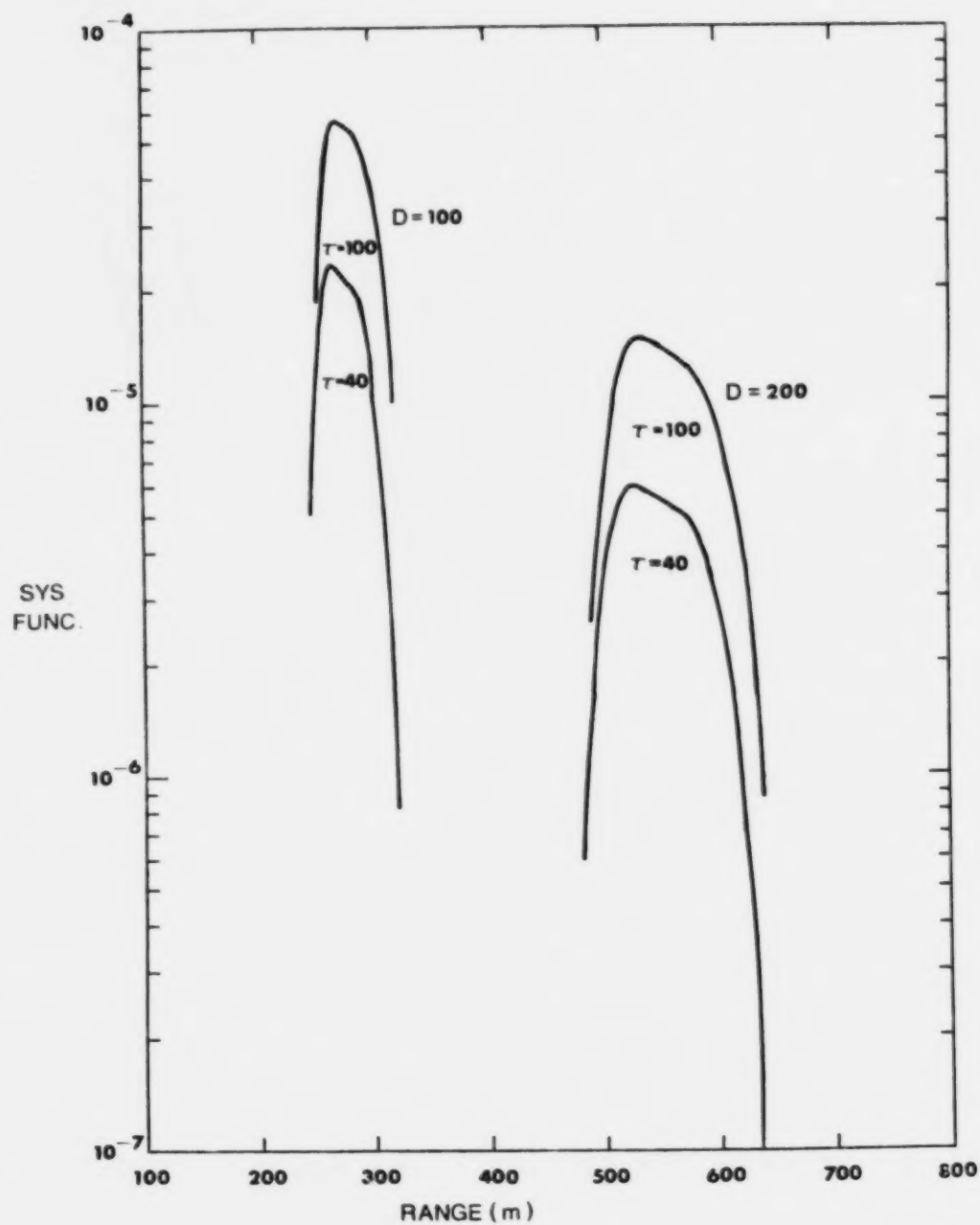


FIGURE 6

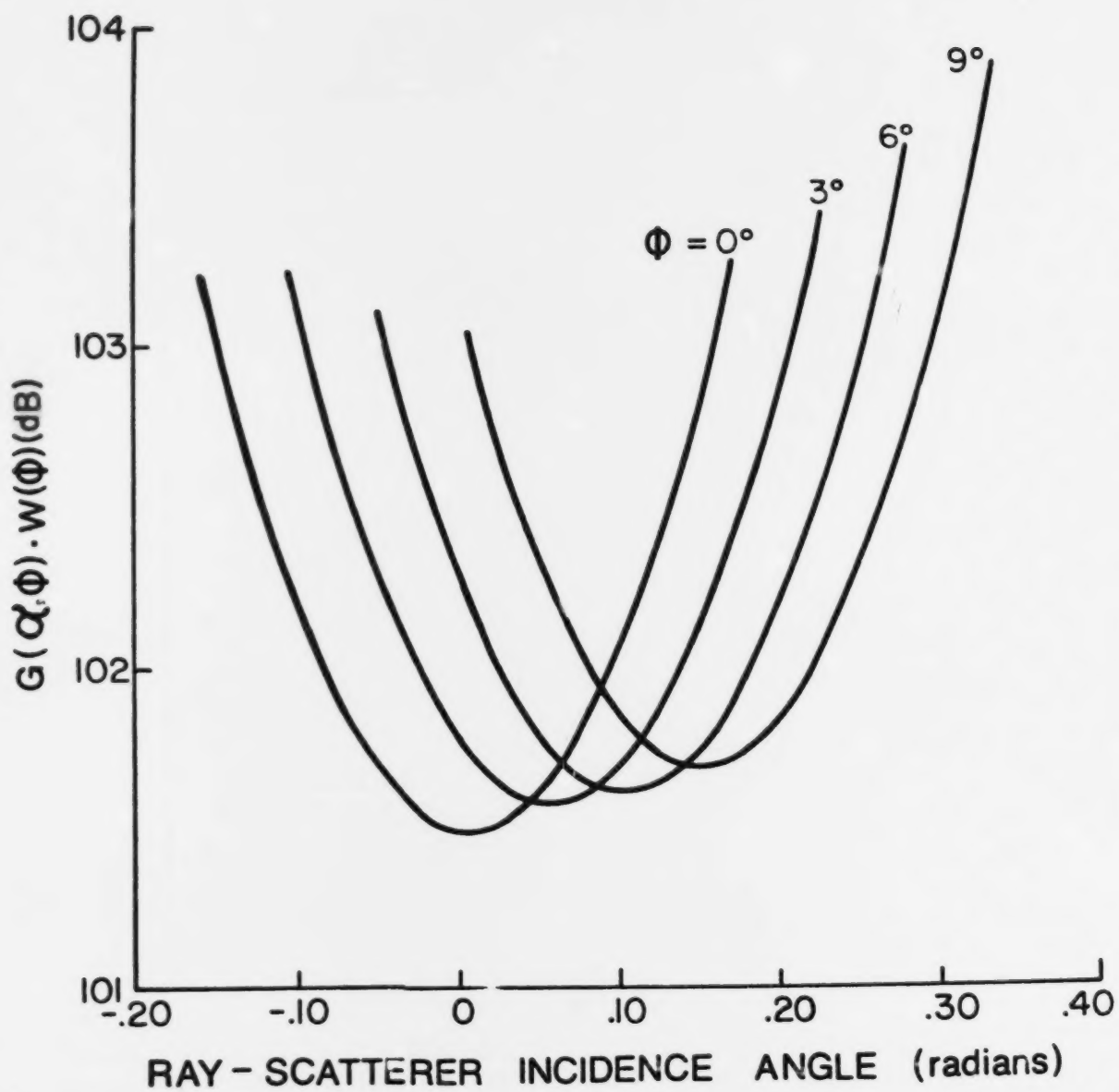


FIGURE 7

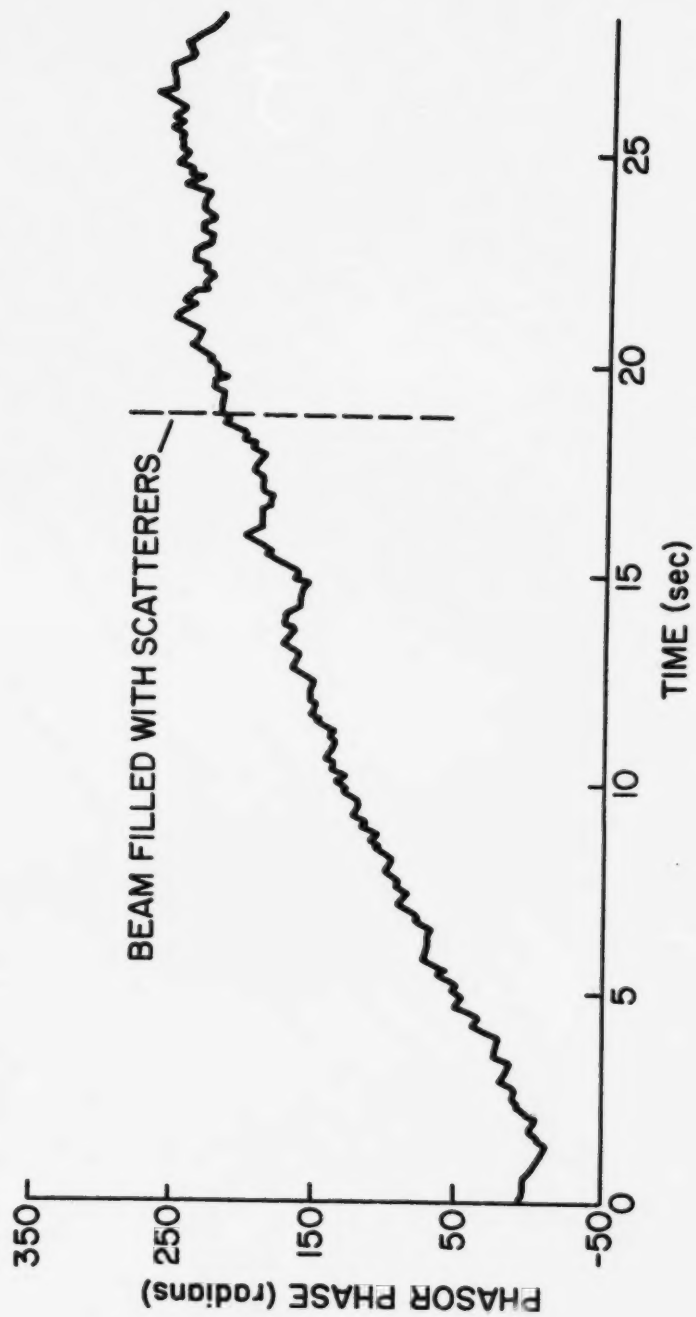


FIGURE 8

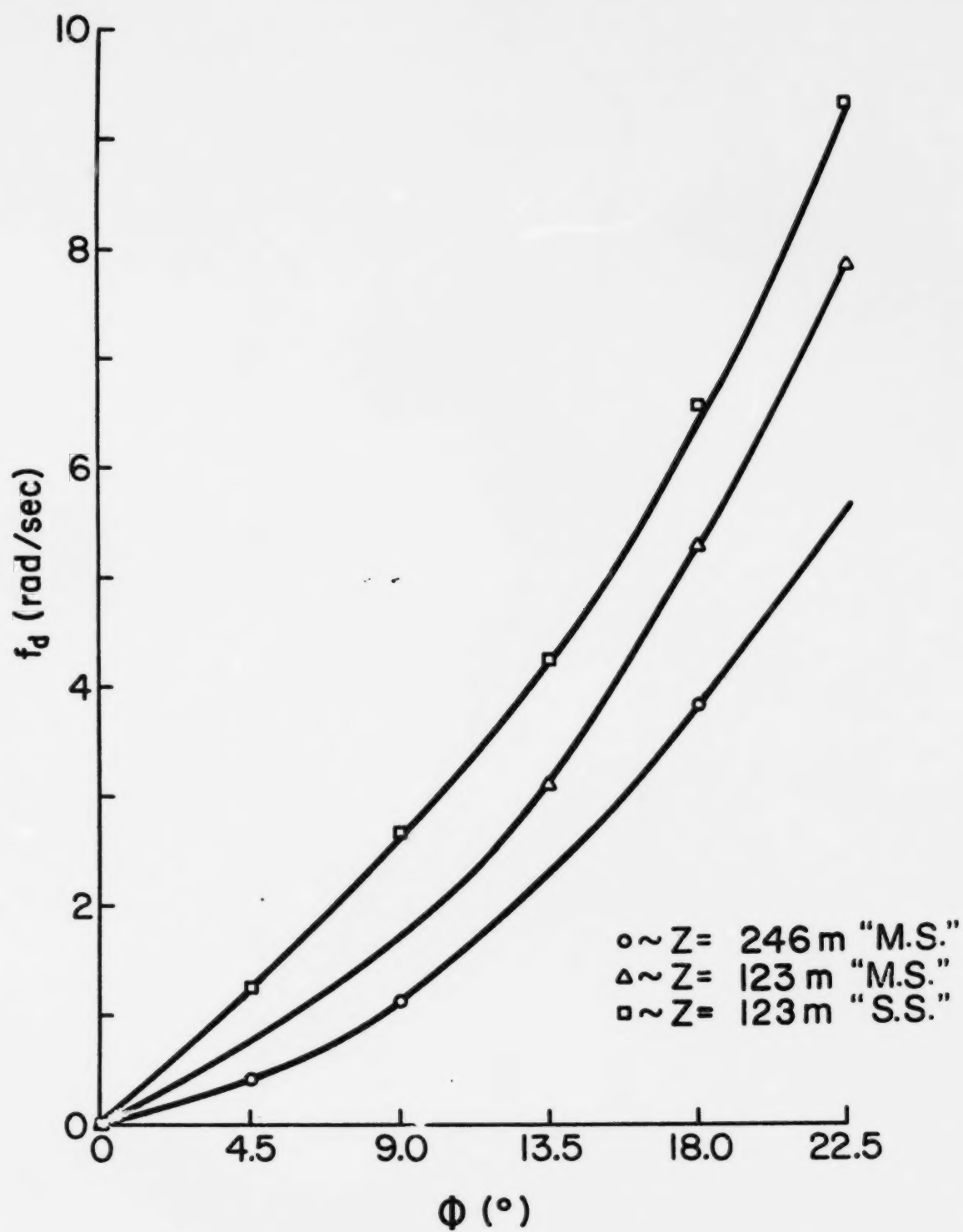


FIGURE 9

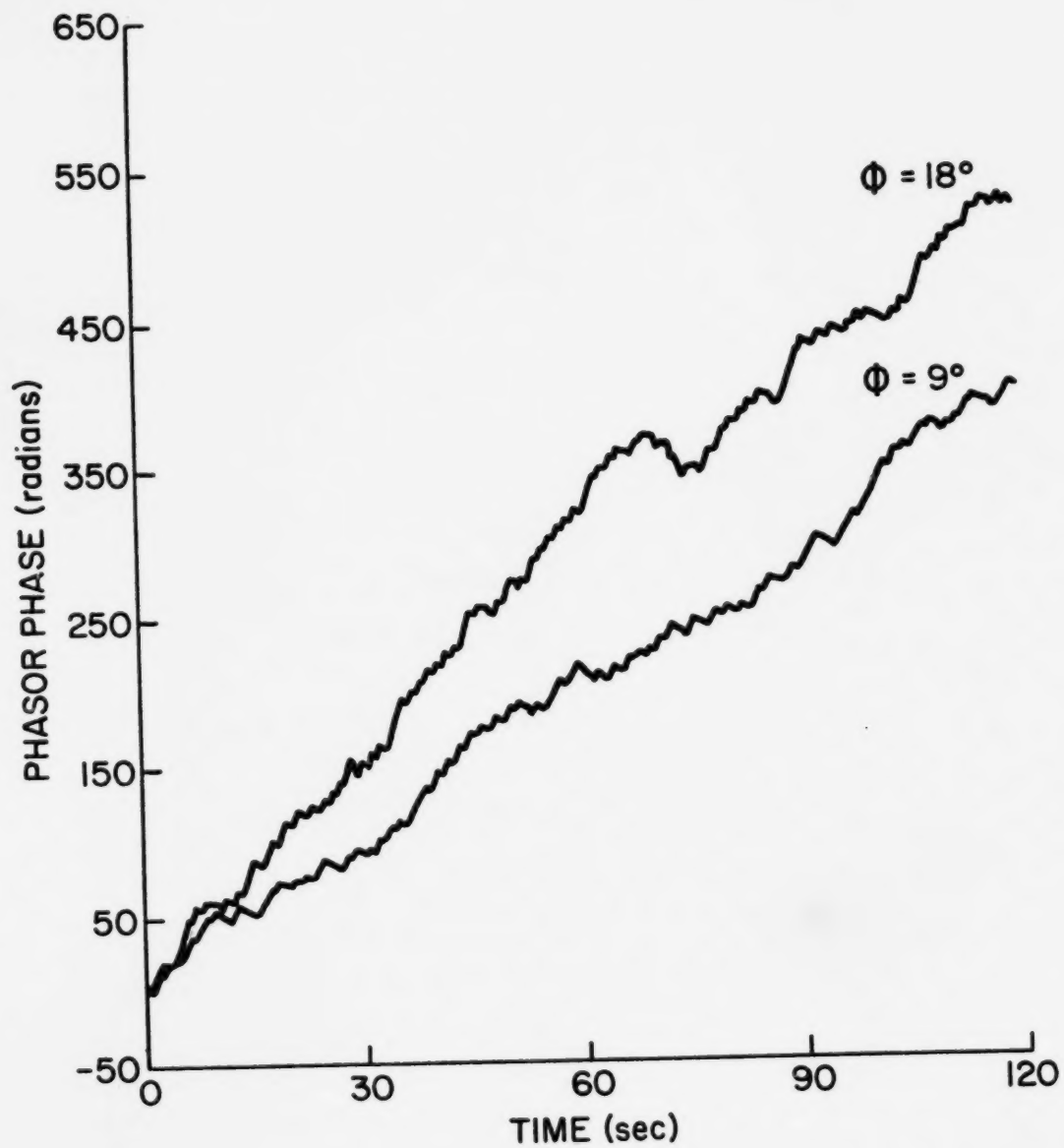


FIGURE 10

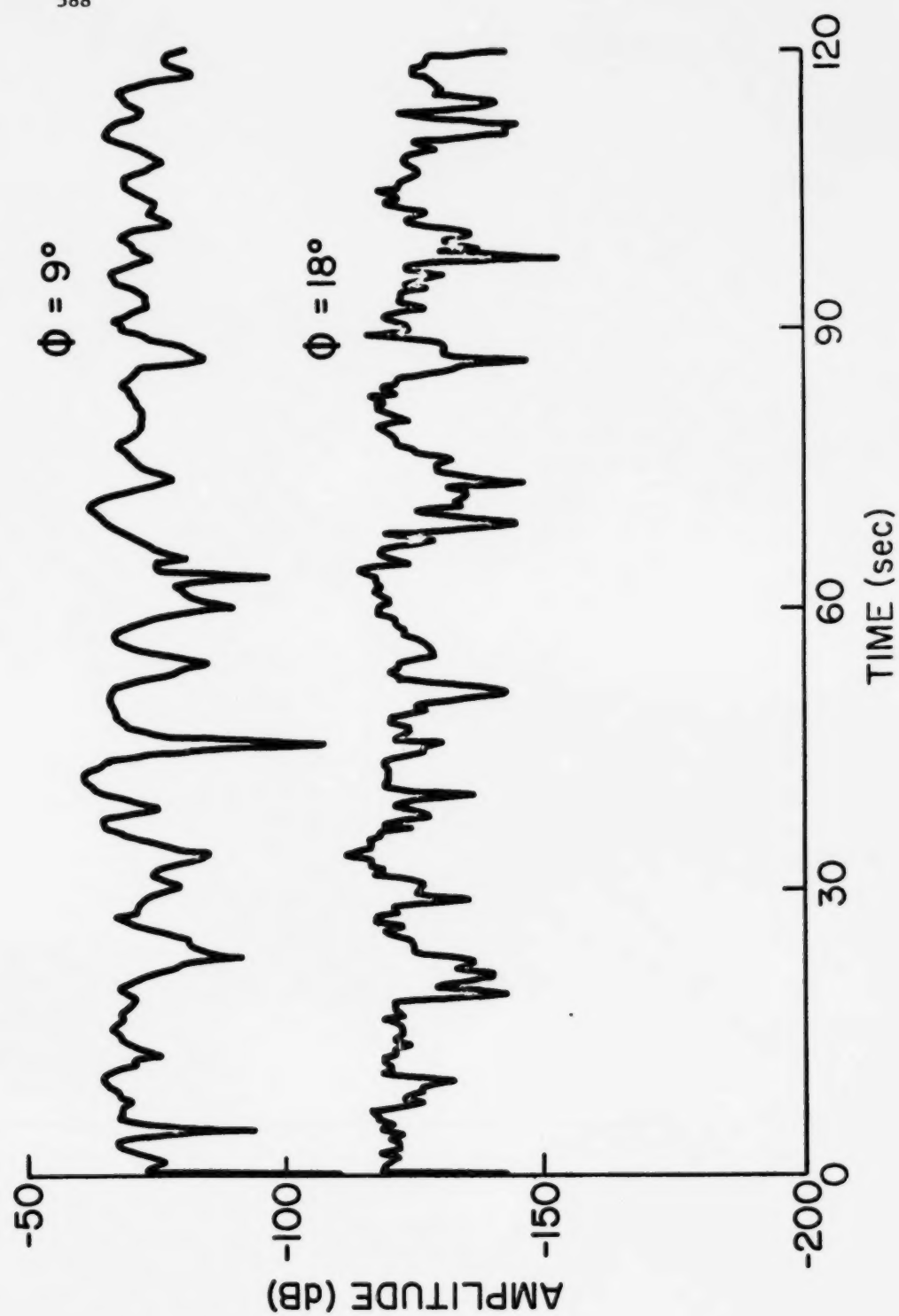
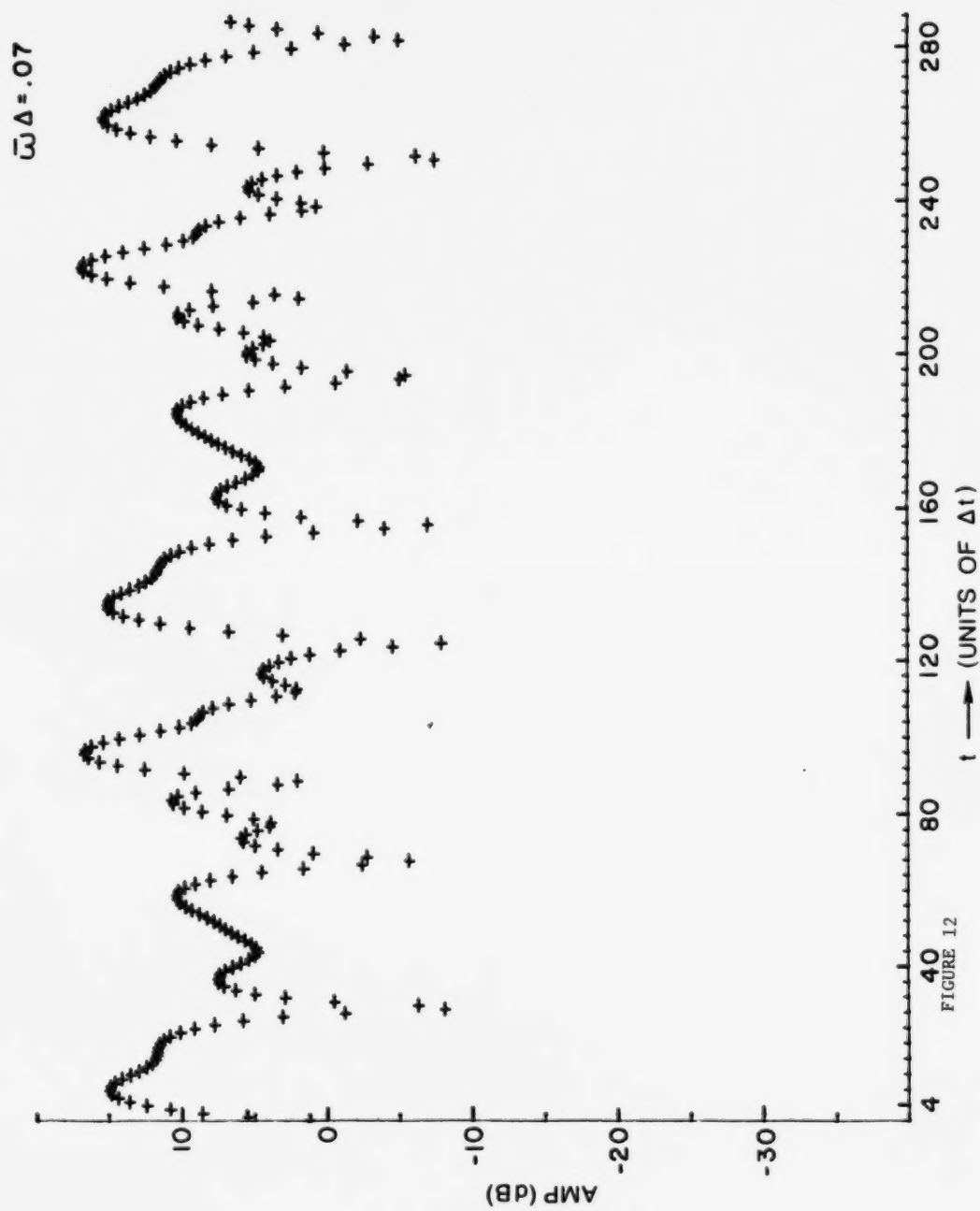


FIGURE 11



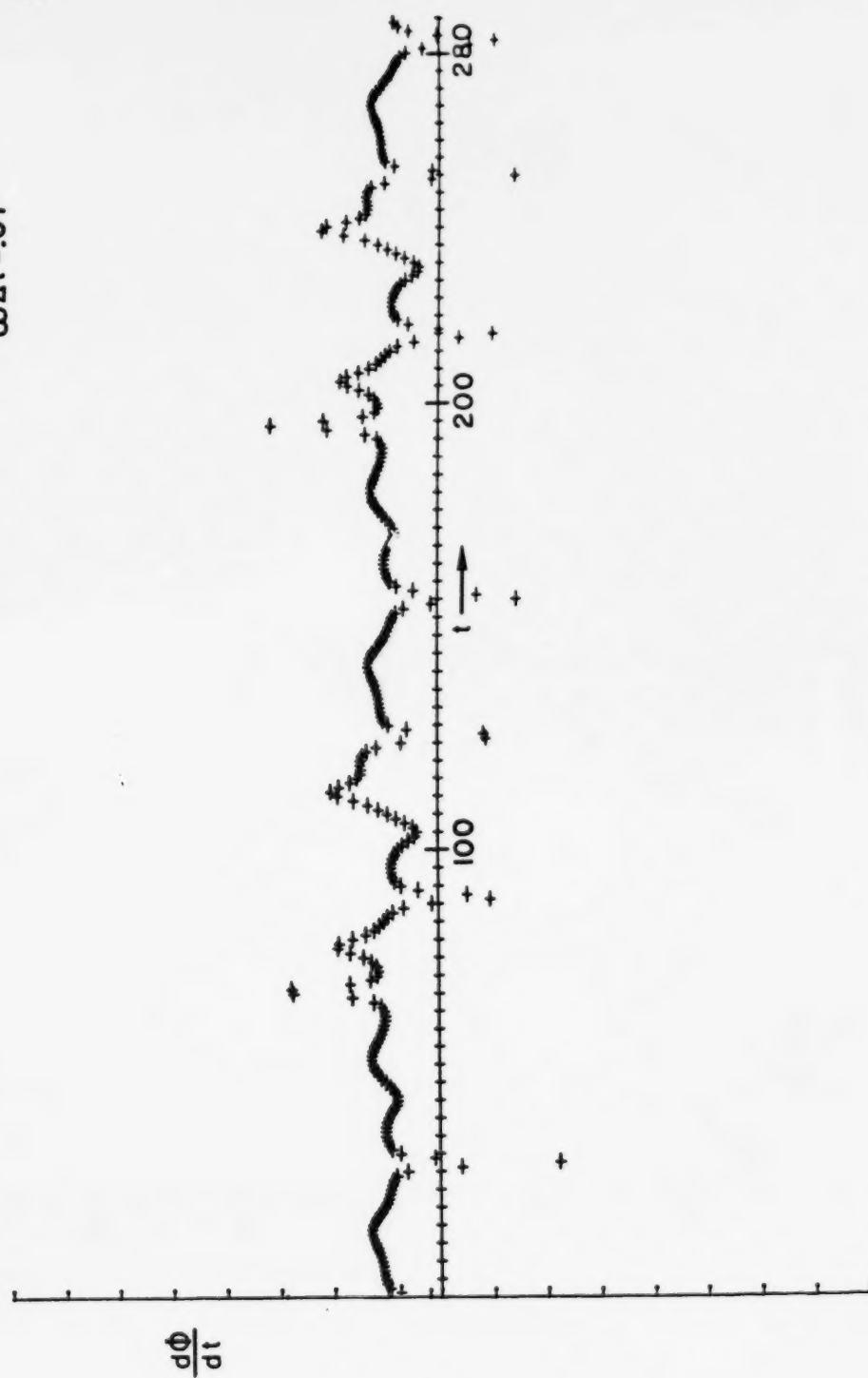
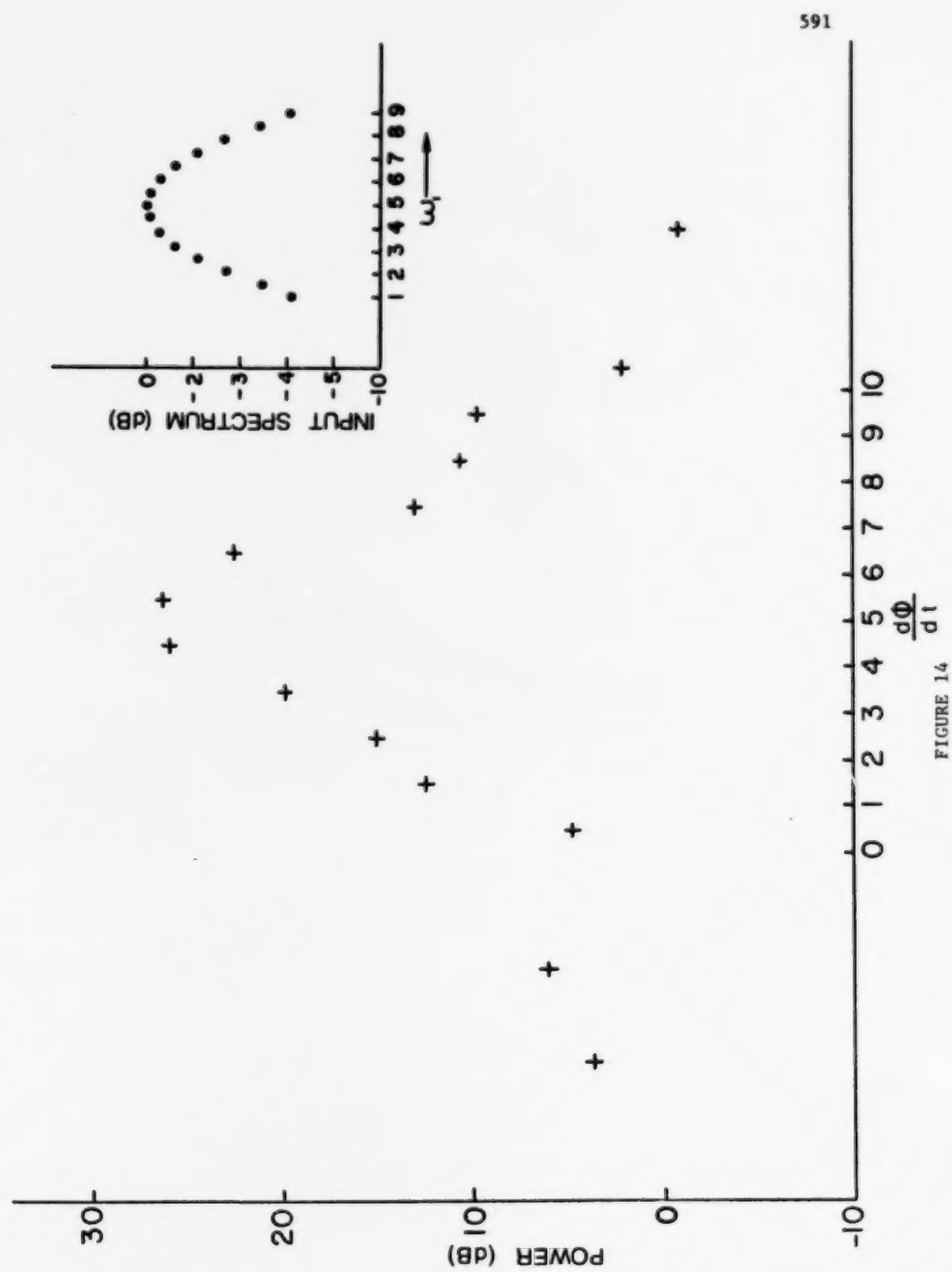
$\bar{\omega}\Delta t = .07$ 

FIGURE 1A



V AIRBORNE MEASUREMENT SYSTEMS

Part 2

1.0 AIRBORNE MEASUREMENT SYSTEMS

D. W. Thomson

1.1 Introductory Remarks

Research in the airborne measurements task group may be conveniently divided into two general areas. In "systems development" we have during the past year, firstly, substantially altered and improved the isokinetic probe for airborne air sampling. Secondly, we have designed, fabricated and tested an airborne radiometer package which includes eight up and down looking hemispherical radiometers with varying wavelength response for use in urban and regional scale energy budget studies. The second general area of research is analysis of a variety of airborne measurements. Turbulence and aerosol observations obtained during the 1973 and 1974 St. Louis RAPS programs and data obtained during the extensive in-house regional measurement program in October, 1973, are serving as the basic data set.

It is important to note that each of the six graduate students participating in the group has not only been assisting in data analysis, but also has through direct participation in the field programs obtained invaluable field measurements experience. Without the combined scientific, engineering and technical expertise contributed by various members of the group, the unique measurements (which for the most part are still being analyzed) discussed in the following sections would not have been possible.

2.0 PSU ISOKINETIC INTAKE FOR AIRBORNE AIR SAMPLING

J. Pena, J. M. Norman and D. W. Thomson

Air pollution studies often require simultaneous measurements of many different parameters. Furthermore, the sampling condition requirements are, in general, different for each sampling instrument. The PSU aircraft is equipped with six different simultaneously operated instruments including particle and condensation nucleus analyzers and an integrating nephelometer. Although it would be preferable to have individual intakes for each of the different instruments, in a medium size aircraft the cost of designing and mounting many parts in the limited available space is prohibitive. Air for each of the instruments could also be sampled from a common chamber where environmental air circulated. However, interpretation of the spatial variation of the air parameters with respect to meteorological variables would then be exceedingly difficult.

For aerosol measurements, especially those concerned with analysis of particle size and distribution, it is very important to sample in isokinetic conditions, that is that air speed at the sampler intake is the same as the air speed across an equal area in the free stream. In order to simplify the adjustment for isokinetic conditions for a particular instrument, it is convenient to have a low air speed (relative to typical aircraft speeds) in the sampling chamber.

A general description of a suitable sampler is as follows: Air enters the sampler through a circular intake and, then, the air speed is

reduced as the cross section increases along a conical section. When the air reaches a cylindrical chamber, its speed is at its minimum value. Behind the sampling chamber, the air (remaining) is again accelerated along a conical section to an end exhaust port.

On board an aircraft truly isokinetic flow can probably not be achieved. A well designed sampler can, however, provide nearly isokinetic conditions. Because of the energy losses at the air intake, along the conical expansion, and at the exhaust, we can expect that the air velocity at the intake will be somewhat lower than the air speed in the free stream. On the other hand, according to Goodale et al (1), the pumping action of the external air stream in passing the exhaust can be enough to compensate the losses and, thus, help to achieve isokinetic conditions.

Another problem with this type of sampler is that when the various sampling instruments are operating, the applied suction can change the operating conditions of the sampler. One way to minimize this effect is to make the primary air flow through the sampler much larger than the combined total flow required by the instruments. Thus, any change in the number of operating instruments will have little influence on the operation of the sampler.

2.1 Design of the PSU Model II Probe

A cross-sectional view of the sampler is shown in Figure 1. In the sampler air is taken through a circular intake of 2.03 cm diameter and its velocity in a conical expander reduced by a factor of 16.6 times before it reaches the sampling chamber.

The flow through the probe is 10 times the flow of the six instruments sampling from it.

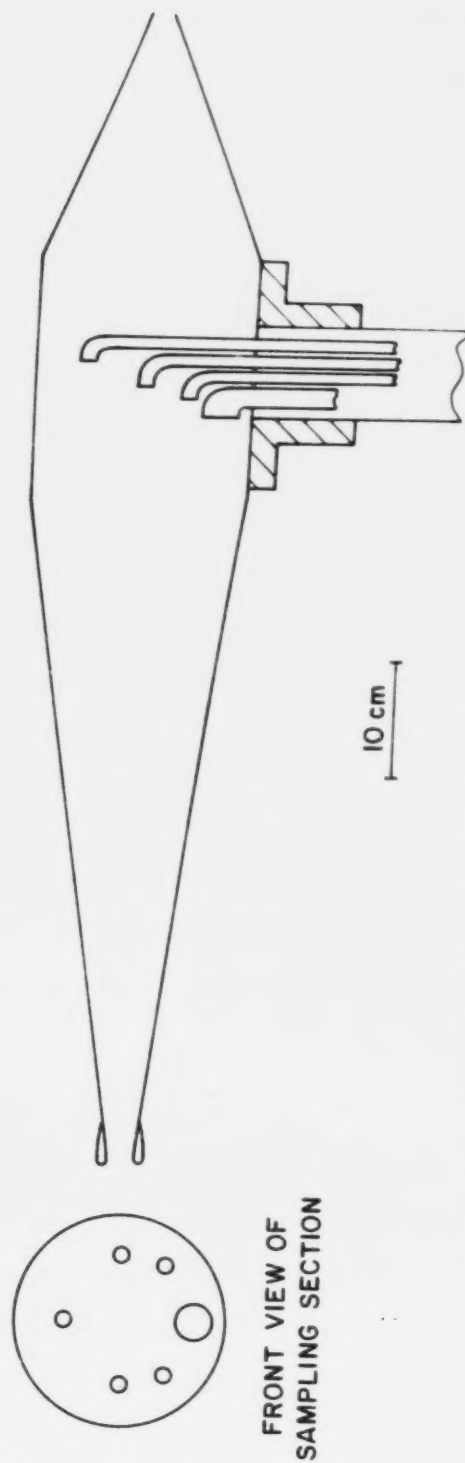


FIGURE 1 : CROSS-SECTION OF AIR SAMPLING PROBE

(a) Air Intake

The air intake profile was designed according to formulas given by Kuchemann and Weber (2) for circular intakes. With the notation of Figure 2 the outer shape is given by

$$\frac{r}{R_m} = \frac{R_o}{R_m} + \left(1 - \frac{R_o}{R_m}\right) \left(1 - \left(1 - \frac{R_m}{L} \frac{x}{R_m}\right)^2\right)^{1/2} \quad (1)$$

and the inner shape by

$$\frac{r}{R_m} = \frac{R_o}{R_m} - \left(\frac{R_o}{R_i} - 1\right) \frac{R_i}{R_m} \left(1 - \left(1 - \frac{R_i}{L_i} \frac{x}{R_i}\right)^2\right)^{1/2} \quad (2)$$

The inner and outer thickness and the lengths of the inner and outer curved portions are given in terms of the area ratio $\frac{A_i}{A_m}$ and the four constants

$$K_1 = \frac{R_o}{R_i} ; \quad \frac{R_o}{R_m} = K_1 \left(\frac{A_i}{A_m}\right)^{1/2}$$

$$\frac{R_m}{L} = K_2 + K_3 \left(\frac{A_i}{A_m}\right) ; \quad \frac{R_i}{L_i} = \frac{1}{K_4 (K_1 - 1)}$$

being the values of the constants:

$$\begin{array}{ll} K_1 = 1.15 & K_2 = 0.2 \\ K_3 = 12.5 & K_4 = 1.5 \end{array}$$



FIGURE 2 : CROSS-SECTION OF SAMPLER AIR INTAKE.

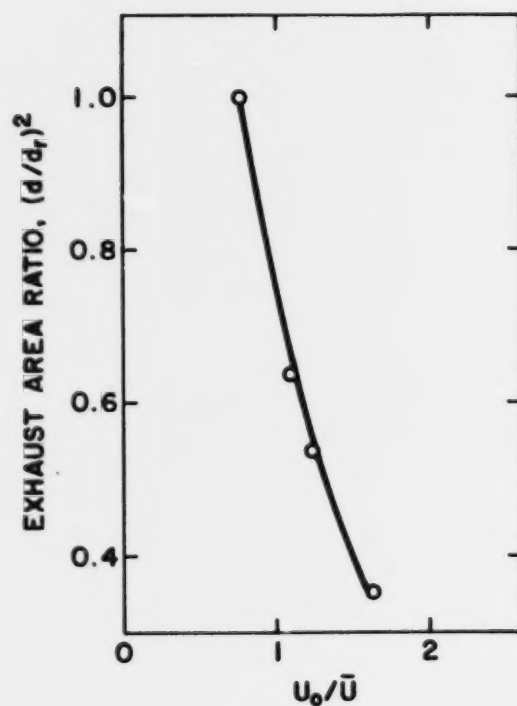


FIGURE 3 : EXHAUST AREA RATIO AS A FUNCTION OF FREE STREAM AND SAMPLER INTAKE VELOCITIES.

For our intake we have taken

$$R_i = 0.89 \text{ cm and } \frac{A_i}{A_m} = 0.25$$

(b) Conical Diffuser

The diffuser has an angle of 7° which minimizes both losses and flow separation. The cone was constructed on a model using polyester resin and fiberglass. The previous model (see 1973 Annual Report) with a cone of 19° exhibited a wind velocity profile within the sampling chamber which indicated a substantial amount of flow separation. The change of cone angle from 19° to 7° reduced the level of turbulence ($\frac{u_{r.m.s.}}{\bar{u}}$) from 0.32 to 0.05.

(c) Sampling Chamber

The sampling chamber is cylindrical in shape with an I.D. of 8.28 cm and a total length of 10 cm. The tubes leading to the individual instruments are located in the area limited by the distances 7.5 cm and 12.5 cm from the entrance to the chamber. There are five 0.635 cm I.D. stainless steel and one 2.54 cm I.D. p.v.c. tubes. Each of these tubes may be individually adapted for isokinetic sampling by using the appropriate size nozzle to match the local air speed in the sampling chamber.

(d) Sampler Exhaust

According to Goodale et al (1) the pumping action of the air stream in passing the exhaust can be used to compensate the losses inside the sampler. They used a value that enabled them to modify the exhaust area.

In wind tunnel tests, we measured the behavior of the sampler as a function of exhaust port diameter. Figure 3 shows a plot of $\frac{u_o}{\bar{u}}$ vs the exhaust area ratio $(\frac{d}{d_t})^2$ where

u_o = air velocity in free stream

$\bar{u}$ = mean air velocity at the sampler intake

d_t = reference exhaust diameter. It is the diameter for which we obtained the lowest test values of $\frac{u_o}{\bar{u}}$.

d = exhaust diameter

2.2 Sampler Performance

The performance of the sampler is characterized by the value of $u_o/\bar{u}$. For $\frac{u_o}{\bar{u}} = 1$ the sampling will be approximately isokinetic. From Figure 3 it can be seen that isokinetic conditions can be obtained with the proper choice of d . The final size is chosen, of course, by measuring the velocity profile within the sampler during test flights.

The value of $\bar{u}$ was determined from the velocity profile in the sampling chamber as measured with a hot wire anemometer. It is given by

$$\bar{u} = v_m e \frac{A_{eff}}{A} \quad (3)$$

where

v_m is the mean velocity in the sampling chamber and it is obtained from the measured velocity profiles

e is air expansion rate inside the sampler

$$e = \left(\frac{R_s}{R_1}\right)^2 \quad (4)$$

being R_s is the radius of the sampling chamber and R_1 that of the intake

A is the area of the geometrical cross section of the sampling chamber

$$A = \pi R_s^2 \quad (5)$$

and

$$A_{\text{eff}} = \pi (R_s - \delta^*)^2 \quad (6)$$

is the effective area.

The displacement thickness δ^* is given by (3).

$$\delta^* = 1.74 \sqrt{\frac{\nu \chi}{v_\infty}} \quad [\text{cm}] \quad (7)$$

being

ν = kinetic viscosity for $\nu = 0.17 \text{ cm}^2 \text{ sec}^{-1}$

χ = distance from the entrance to the chamber $\chi = 10 \text{ cm}$

v_∞ = air velocity at the center line of the chamber in cm/sec^{-1}

Taking into account (3), (4), (5), and (6), we obtain

$$\frac{u_o}{\bar{u}} = \frac{u_o R_1^2}{v_m (R_s - \delta^*)^2} \quad (8)$$

From (8) it can be seen $\frac{u_o}{u}$ depends mainly on v_m .

There are two circumstances we have carefully checked:

- (1) How v_m changes when u_o changes
- (2) How v_m changes when the sampler is tilted from the horizontal position

(a) Influence of u_o on v_m

The sampler was thoroughly wind tunnel tested at a wind speed of 46 m/sec. (the tunnel's maximum). Although the aircraft speed when sampling is 62m/sec, this difference in wind speed is not important because the performance of the intake ($u_o/\bar{u}$) is not affected by a change in the Reynolds number once it exceeds about 3000.

Thus, we expect that $\frac{u_o}{v_m}$ will remain constant.

Measurements of $v_m = f(u_o)$ were made with the sampler installed in the aircraft for u_o in the range 40 to 81 m/sec. Measurements in the wind tunnel at 42 m/sec fit well with those obtained in the aircraft.

(b) Dependence on tilting of the sampler

The value of v_m was measured in the wind tunnel with the sampler in the horizontal position and tilted 8° (the maximum expected attack angle variation) from the horizontal. The results indicated negligible sensitivity to angle of attack.

2.3 Conclusions

Although a few final airborne tests for the sampler are planned, it has been installed in the aircraft and was successfully used during the August, 1974, St. Louis measurements.

According to the wind tunnel tests

$$\frac{u_o}{u} = 1.18$$

Although this value is certainly very close to being correct, we do want to better determine in normal flight conditions how exhaust size affects the sampler efficiency.

3.0 INSTRUMENTATION FOR MULTIWAVELENGTH AIRBORNE PRECISION SPECTRAL RADIOMETER MEASUREMENTS

J. M. Norman, D. W. Thomson, W. Benson, J. P. Breon

At the request of the EPA Meteorology Laboratory, a capability of measuring hemispherical radiation in four wavelength bands, from 0.295 μm to 60 μm , has been added to the existing Pennsylvania State University aircraft instrumentation system. Eight Eppley radiometers (to monitor both upward and downward radiation streams) have been mounted on the aircraft. The radiometers are interfaced to the existing data logging system through individual especially constructed preamplifiers so that signals from all eight may be sampled at up to twice per second.

3.1 The Radiometers

Six Eppley, Model 2, precision spectral radiometers (PSR), sensitive in three wavelength bands of the solar spectrum, have been obtained from the EPA expressly for mounting on the aircraft, and two Eppley precision infrared radiometers (PIR) have been purchased to facilitate measurements in the wavelength band from 4 to 60 μm . Thus the wavelength band from 0.295 to 60 μm is partitioned into 4 regions: (1) 0.295 - 3 μm , (2) 0.395 - 3 μm , (3) 0.695 - 3 μm and (4) 4 to 60 μm . Three PSR's and one PIR are mounted facing upwards to measure the downward directed irradiance and a similar complement is mounted facing downwards to sense the upward radiation stream. Figure 1 shows the spectral transmittances for the

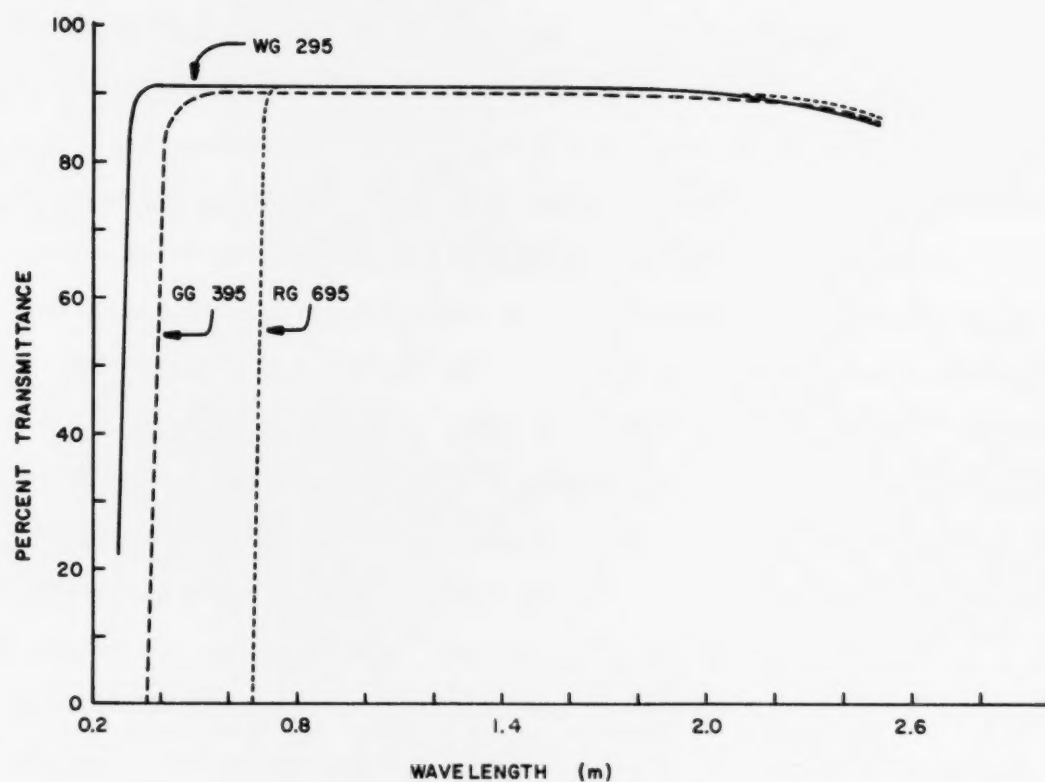


FIGURE 1: SPECTRAL RESPONSE OF EPPLEY MODEL 2 DOMES

domes of the various pyronometers as published by the Eppley Corporation.

The spectral response of the pyrgeometer is described as follows:

"The composite envelope transmission exhibits a sharp transition between about 3 and 4 μm , from complete opaqueness to maximum transparency, and (apart from the normal waviness associated with such interference patterns) a general transmittance of about 0.50 decreasing, with increasing wavelength, to 0.30-0.40 around 50 μm ."

The calibration factors provided by Eppley were checked with a Link-Fuessner pyrhelimeter recently acquired by the Meteorology Department. On a clear day the Link-Fuessner is used to determine the solar beam flux density (in a plane perpendicular to the direction of the sun) and at the same time a PSR is shaded with a paddle that is designed to obscure the same solid angle as the Link-Fuessner views. After accounting for the sun incidence angle, which is calculated from true solar time (as well as measured with the Link-Fuessner), the difference between the total output (unshaded) and the diffuse only output (shaded) should correspond to the flux density indicated by the Link-Fuessner. Zero drifts on all radiometers must be carefully monitored if 1% accuracy is to be obtained. The pyranometer with the RG695 is subject to particularly large zero shifts (often greater than 4%) under high radiation conditions with light winds due to heating of the outer dome by the absorbed visible radiation. This is likely to be completely negligible during operation on the aircraft. Since only a RG695 filter (calibrated) was available with the Link-Fuessner, it was not possible to check the PSR with the GG395 dome by this technique. However, each of the pyronometers was checked by a second method that involved comparison with a reference pyronometer (serial no. 12699F3). The WG295

**TABLE 1: RESULTS OF EPPLEY MODEL 2 CALIBRATIONS THAT WERE
CONDUCTED AT THE PENNSYLVANIA STATE UNIVERSITY IN 1974.**

RADIOMETER SERIAL NO.	FILTER DOME	CALIBRATION FROM EPPLEY CORP.		CALIBRATION WITH LINK JUNE 9		CALIBRATION WITH WG 295 ON EACH RADIOMETER JUNE 10 - RATIO TO # 12699F3
		$\frac{mv - min}{Ly}$	RATIO TO #12699F3	$\frac{mv - min}{Ly}$	RATIO TO #12699F3	
12699 F3	WG 295	6.79	1.000	6.74	1.000	1.000
12698 F3	WG 295	6.92	1.019	-	-	1.017
12708 F3	RG 695	6.97	1.027	7.08	1.050	1.025
12709 F3	RG 695	7.15	1.053	7.20	1.068	1.053
12623 F3	GG 395	5.97	0.879	-	-	0.880
12624 F3	GG 395	5.69	0.838	-	-	0.835

TABLE II: SPECIFICATIONS FOR EPPLEY PRECISION SPECTRAL RADIOMETER (PSR) AND PRECISION INFRARED RADIOMETER (PIR).

<u>SPECIFICATION</u>	<u>PSR</u>	<u>PIR</u>
IMPEDANCE	300 OHM	400 OHM
TEMPERATURE COEFFICIENT	$\pm 0.5\%$ - 20°C TO +40°C	$\pm 0.5\%$ - 20°C TO +40°C
TIME CONSTANT	1 SEC.	2 SEC.
COSINE RESPONSE	$\pm 1\%$ 10° - 90°	< 5%
LINEARITY	< 1% TO 4 Ly/min $\pm 1\%$ TO 1 Ly/min	
ORIENTATION	NO EFFECT ON INSTRUMENT PERFORMANCE	
MECHANICAL VIBRATION	WITHSTAND UP TO 20 g's	

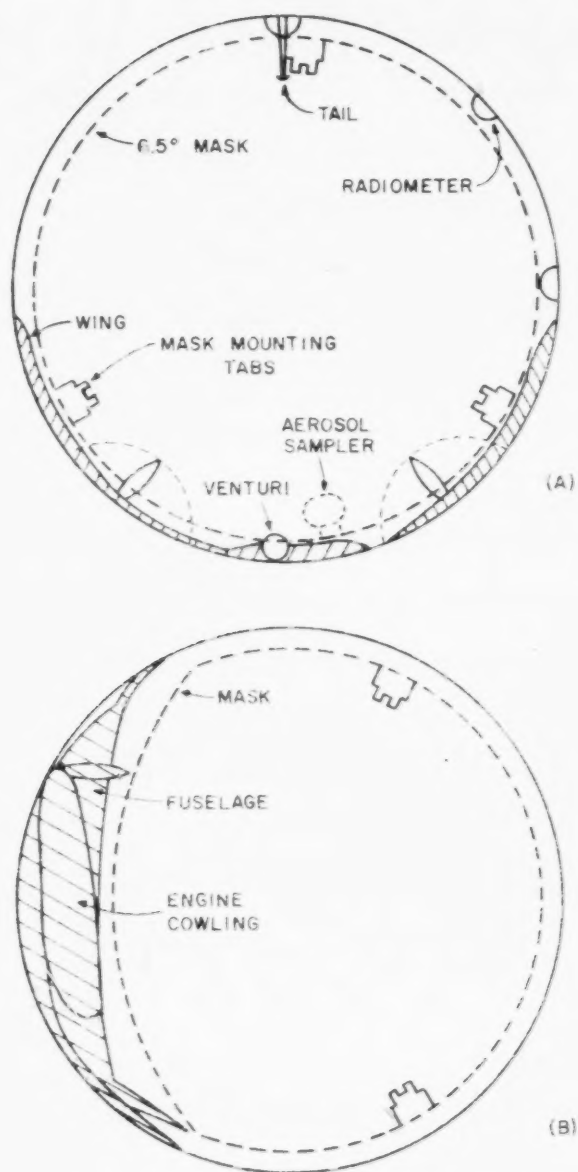


FIGURE 2: HEMISPHERICAL VIEW OF (A) UPWARD FACING AND (B) DOWNWARD FACING RADIOMETERS WHEN MOUNTED ON THE AIRCRAFT.

dome from pyranometer number 12698F3 was installed on each radiometer, and one at a time the output of each PSR was compared to the reference PSR. All of the calibration results are contained in Table. 1. The PIR's are more difficult to calibrate and Eppley's calibrations were not checked except to insure that they gave reasonable readings in a cavity of known temperatures. At the present time, a calibration cavity is being designed so that more precise calibration can be obtained.

The angular response of the radiometer is sufficiently close to an ideal cosine response so that negligible errors occur in hemispherical readings because of improper angular response. However, on some occasions, it may be desirable to restrict the view of the downward facing radiometers to something less than a full hemisphere. To facilitate this, blackened cylinders have been fabricated to restrict the radiometer view to within $\pm 30^\circ$ of a perpendicular through the center of the thermopile surface. These cylinders also have tops and, thus, otherwise, serve as protective covers for the radiometer domes. The top of the PIR cylinder also has provision for a dessicant to prolong the life of the KRS-5 dome.

A brief summary of the specifications of the PSR and PIR is contained in Table 2.

3.2 Radiometer Mounting

The eight radiometers were mounted on the aircraft with four facing upwards (fuselage mount) and four facing downwards (starboard wing mount). Both the upward and downward mounts are designed so that the plane of the thermopile is level when the aircraft is in its normal flying altitude, which is $\approx 5^\circ$ nose-up. This requires a carefully designed "double-angle" shim for the wing mounts.

When mounting radiometers, it is most desirable not to have any unwanted structures in the radiometer view. Unfortunately, this is not possible on the Aerocommander so we have dealt with it in a way that allows us to correct for existing blockage. The upward facing radiometers view the top of the wings and forward fuselage, propellers, tail, aerosol sampler, venturi and the other radiometers. The fuselage and wing, which are painted white, constitute the greatest potential source of error so a blackened shadow band has been added to each radiometer to black the radiometer view within 6.5° of horizontal, Fig. 2a. This also blackens most of the venturi as well as the other radiometers. The aerosol sampler and venturi are painted black and the extremely small area of view occupied by propellers and tail is corrected for. Furthermore, it is highly unlikely that the sun could glare from one of these surfaces (those that protrude above the shading band) and the view lost by blackening out these structures is simply not worth the effort which would be required. Glare that finds its way to the thermopile by reflection from the dome also is likely to be negligible.

The downward facing radiometers are mounted below the wing instead of on the lower fuselage for several reasons: (1) It is not necessary to develop elaborate shielding to protect the radiometers during take off and landing. (2) The radiometer domes will be very much easier to keep clean since no oil spray exists as under the fuselage. (3) Suitable mounting points already existed on the starboard wing. The only disadvantage to the wing location is that a substantial fraction (about 13%) of the radiometer view is occupied by the fuselage. Thus, a special blackened mask has been designed to blacken the aircraft structure from the view of the radiometer, Fig. 2b.

This was accomplished by mounting a camera in the precise position of the radiometers, and then photographing their effective view through a hemispherical lens.

Since downward facing pyranometers sense only reflected radiation, which is much smaller than the downward incident radiation, it is very important that no glare from the sun strike the domes or thermopiles. With the shade of the wing and the fuselage blocked by the blackened mask, there is no chance of this happening except at extremely low (few degree) sun angles.

3.3 Radiometer Signal Conditioning

Expected radiation values will usually produce full scale pyranometer output voltages ranging from 30 microvolts to 12 millivolts. With the low irradiance values, particularly in the infrared, it is also desirable to maximize the readout resolution of the records. Normally, to satisfy such requirements, a commercially available, low drift, high gain amplifier system could be used for each pyranometer.

Because the pyranometers had to be physically installed far enough from the aircraft's surfaces to prevent blockage which would have jeopardized the accuracy of the radiation values obtained, the downward looking radiometers were mounted out on the wing approximately 20 feet from the main instrumentation and data acquisition console, and the upward units on the main fuselage about 10 feet from the acquisition console.

This installation posed several major problems in signal conditioning since some of the pyranometers were expected to have very low radiation values. These values had to be transmitted back noise free to the main data console for further conditioning and recording. Furthermore, for the low radiation values, an extended readout resolution or span was necessary to prevent any system sensitivity involvement in the recording process. The final span chosen for each radiometer yields the maximum possible number of counts and accuracy for data reduction.

The low level radiation values required that the amplifier circuits be located near the radiometers to prevent noise generation and signal losses which can be caused in transferring low signal levels over long lines. For the wing installation, airflow considerations had to be made to account for possible influence of temperature variations during flight on the electronic circuits. Space was another prime consideration because of the aircraft wing and inspection plate (which provides wing access) size. Finally, cabling was a major concern. It is always desirable to keep the number of wires to a minimum in such installations to prevent ground loops, excessive weight, and signal interference from other operational systems.

Consultations were made with other research groups and companies that had been involved in the construction and use of analogous instruments. Most groups recommended that improvements to their systems or changes could be made to obtain a more reliable and stable system. This prompted our group to investigate several possible novel circuits.

A study was made of each of the various analog operational amplifier circuits which could be used to provide the gain and stability required in the air flight environment. The list included chopper stabilized, FET, and instrumentation operational amplifiers. A test procedure which included short circuit, open circuit and constant voltage settings over the expected range of operation was established to compare all these circuits. The units were all simultaneously evaluated in a laboratory temperature controlled chamber. With some further studies, an additional circuit was included for evaluation. It consisted of a two wire transmitter circuit as shown in Fig. 3.

The amplifier is a linear integrated circuit designed to convert the voltage obtained from the sensor into a current, and send it through to a receiver, utilizing the same simple twisted pair as the power supply. Use of the power supply leads as signal transmission leads eliminates two or three extra wires for each amplifier. Furthermore, current output minimizes susceptibility to voltage noise spikes and also eliminates line drop problems.

Fig. 4 is a plot of the test results of the amplifiers compared. Observe that the two wire transmitter provided the best stability in the desired range of operation (under the test conditions instituted). This unit was also the simplest to construct and required the least space. Most importantly, it only needed 2 wires to transmit both the power and the radiation signal value to the data console, and thus, it was not necessary to install additional cables in the aircraft wing.

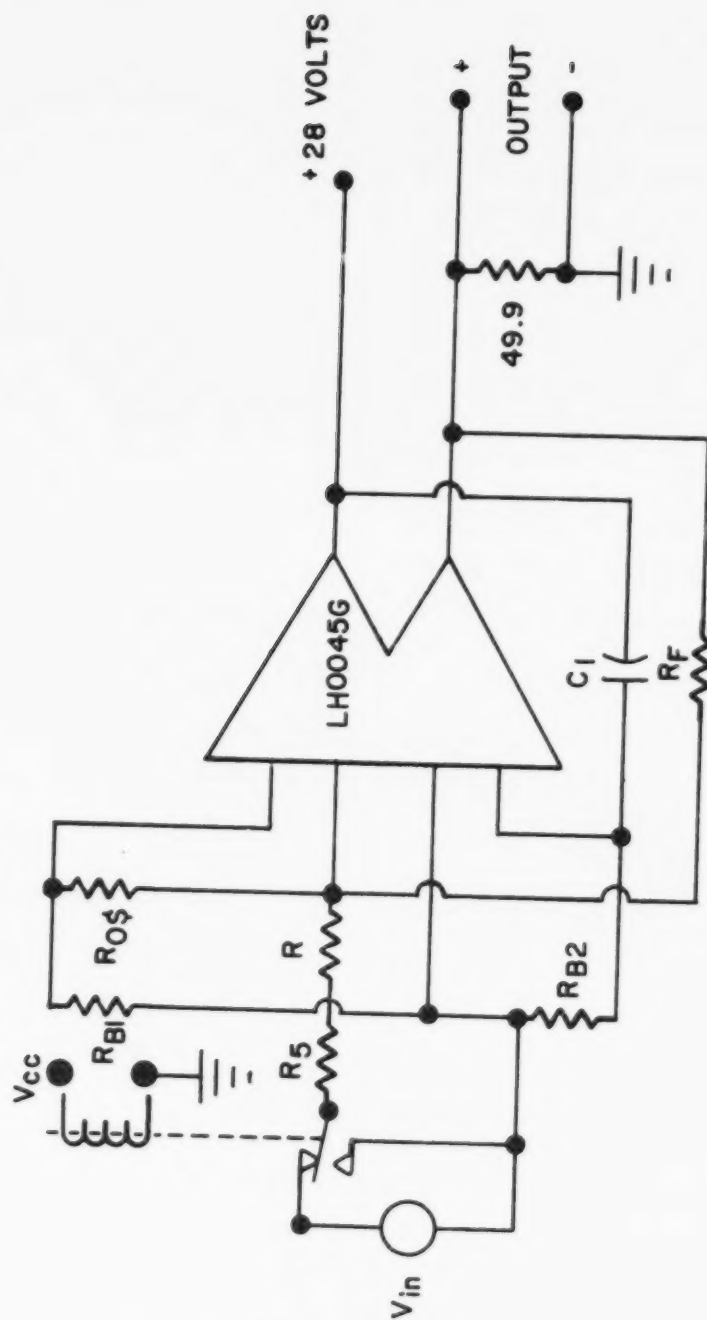


FIGURE 3 : BASIC TWO WIRE CURRENT TRANSMITTER
CIRCUIT

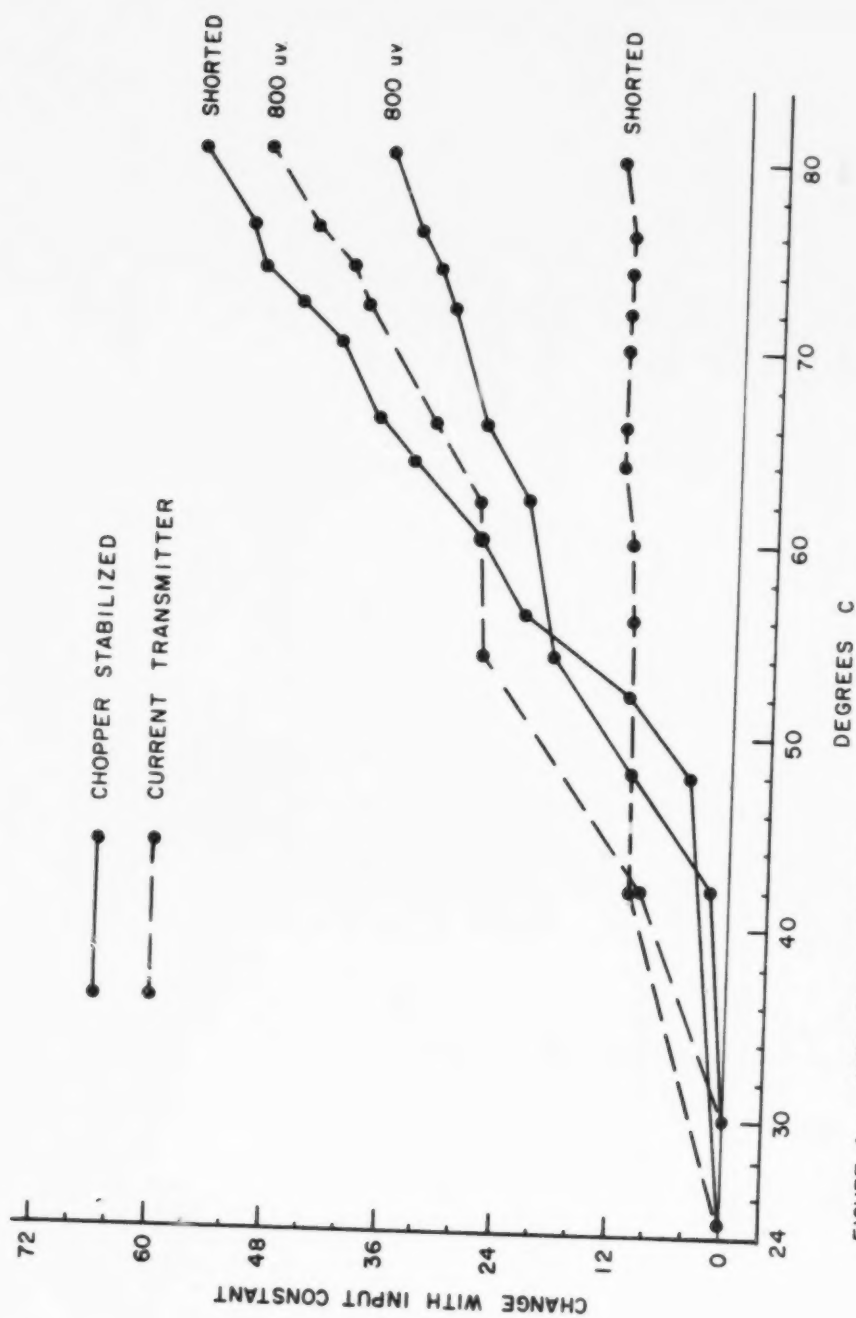


FIGURE 4 : AMPLIFIER STABILITY AS A FUNCTION OF TEMPERATURE .

The total error for a 2 wire transmitter is:

$$\frac{\Delta I_S}{I_{\text{span}}} = \Delta V_{\text{ref}} + \Delta V_{\text{os}} + \Delta R_g$$

where:

I_S = open loop supply current

I_{span} = change in output current from 0% to 100%

V_{ref} = reference voltage regulation

V_{os} = input offset voltage

R_g = current setting resistor

Typical values for our conditions were approximately 0.45%. To assist in constant evaluation of this error an auto ground reference system was incorporated into the installation. It provides checks for temperatures and zero drift which can then be corrected in data reduction. The two wire transmitter has an operating voltage range from 10 to 50 volts DC which allowed use of the aircraft supply voltage. This prevented further drain on other instrumentation power supplies or the installation of new supplies. Lastly, the transmitter unit is capable of gains up to 1500 with the same stability factor -- an important feature in this type of operation.

The output of the two wire transmitter is fed to the extender circuit shown in Fig. 5. This circuit has an operational amplifier that has a voltage divider and adjustable input compensation network. The circuit, with all its possible gain and output adjustments enabled full range coverage

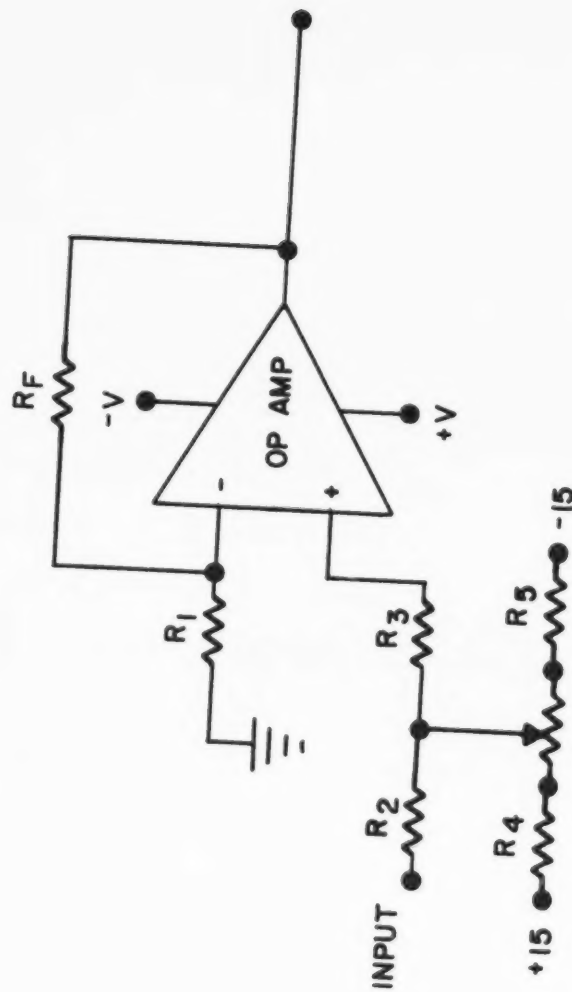


FIGURE 5 : EXPANDER AND POSITIONING CIRCUIT

from all of the radiometer output signals to cover a full ± 1 volt input range for data recording. A complete calibration procedure has been developed for the two wire transmitter. It is reasonably easy and can be accomplished with available standards for signals of this level and type.

3.4 Correction of Radiometer Outputs

The task of correcting the output of a radiometer due to obscured portions of its view requires that the radiant intensity in the portion of view in question be known. For this reason a blackened mask (using 3M velvet black paint) is used to obscure the view so that negligible amounts of pyranometer signal arise from this region and so that the thermal emissivity of this region is known for correction of the PIR. The total flux density received by a cosine-compensated sensor can be written

$$E = \frac{1}{\pi} \int_0^{\pi/2} \int_0^{2\pi} I(\theta, \phi) \sin \theta \cos \theta d\theta d\phi$$

where θ is the angle from the normal to the sensing surface and ϕ is its orthogonal counterpart for spherical coordinates, $I(\theta, \phi)$ is the radiant intensity and E the flux density. The sensor output arising from the incident energy is cE where c is the calibration factor (mv/Ly/min). If the illuminated hemisphere is assumed isotropic, which certainly is reasonable since the view corrections are small anyway, the fraction of the sensor view arising from any region of the hemisphere is

$$f = \frac{1}{\pi} \int_{\theta_1}^{\theta_2} \int_{\phi_1}^{\phi_2} \sin \theta \cos \theta d\theta d\phi$$

$$= \frac{(\phi_2 - \phi_1)}{2\pi} [\sin^2 \theta_2 - \sin^2 \theta_1]$$

If the output, which arises only from diffuse radiation, from a partially obscured pyranometer is V_1 and f is the fraction of the hemispherical view blocked, then the corrected voltage is given by $V_c = V_1/(1-f)$. Correction of the PIR output is more difficult because the temperature of the obscured region must be known. The output of the PIR thus has contributions from two sources; the surface of interest and the shield. Again assuming isotropy of the diffuse angular distribution, the true flux density arising from the underlying surface and corrected for the effect of the shield becomes

$$\frac{V_c}{c} = \left[\frac{V_1}{c} - f\sigma T_s^4 \right] / (1-f)$$

where T_s is the shield temperature (probably very near the measured air temperature), σ is the Stephan-Baltzman constant and V_1 is the actual voltage recorded from the partially obscured radiometer. For the upward facing radiometers $f = 0.022$ and for the downward facing $f = 0.136$.

A precise view factor correction for the upward facing pyranometers requires separation of beam and diffuse components of the irradiance; however, the total correction is so small that values accurate to 1% can

be obtained by using $f = 0.01$ for all conditions. Using $f = 0.01$ may also be most reasonable under overcast conditions since it is well known that an overcast sky is brighter near the zenith than near the horizon. Under hazy conditions when direct beam and diffuse components may be comparable, using $f = 0.01$ is likely to be most suitable.

3.5 Data Analysis

When direct beam radiation from the sun is the major contributor to downward irradiance, for instantaneous readings it may be necessary to correct the radiometer outputs for changes in aircraft altitude. In the PSU aircraft altitude angles are available from gyroscopes, however, corrections should not be necessary if averages over substantial periods are desired.

When the aircraft passes over discontinuities in terrain, the radiometers will lag behind the actual irradiance change because of their time constants. Some of this information can be recovered by reconstruction the time series using the known time constant of the instrument (see Dutton, 1962, and Bauer and Dutton, 1962). Although the radiometer system has already been used for urban energy budget studies in RAPS, several tests do remain to be conducted. They include zero shifts under rapidly changing air temperature conditions and calibration runs over relatively homogeneous surfaces such as a large lake.

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4.0 AIRBORNE MEASUREMENTS OF TURBULENCE

IN THE PLANETARY BOUNDARY LAYER

T. G. Redford, M.S. Thesis Research in Progress

During the past two years, a comprehensive series of aircraft flights to measure the statistical properties of turbulence in the planetary boundary layer have been conducted under a variety of conditions. They have been flown during all four seasons, day and night, over urban and rural areas, and over mountainous and flat terrain. Most of the flights have been in neutral or unstable weather conditions, clear of clouds and precipitation, during the day and over or near the city of St. Louis, Missouri. Many of the flights were coordinated with other research efforts underway in the EPA RAPS program. Altitudes for the observations ranged from 1000 feet above the surface to 9,500 feet, but measurements below 5,000 were emphasized. We quickly established that there was little point in attempting to measure turbulence at night or in stable low wind conditions. The aircraft turbulence system lacked sufficient sensitivity to resolve the low levels of turbulence existing under those conditions.

The properties of boundary layer turbulence are affected by the inter-relation of many factors including wind speed, stability, topography and altitude. Therefore, our efforts to analyze the turbulence have been made by statistical analysis of each related independent and dependent parameters. As the measure of turbulence, the vertical wind speed is used because we expect the scale of the vertical gusts to be on the same order

of magnitude as that of air motion usually referred to as turbulence. In order to compute the vertical gust velocities, we combine outputs from the following sensors:

P = static pressure

T = temperature

IAS = indicated air speed

$\dot{W}_{ac}$ = vertical acceleration

Θ = pitch angle

ΔP = pressure difference between upward and downward oriented impact pressure probes

Additional information such as Doppler winds was recorded for navigation purposes and to allow for future analysis of more subtly related factors.

The output from each respective transducer, converted to an electrical signal, is fed into a multichannel Analog-to-Digital Converter. All signals are scanned twice per second, converted to a digital format and recorded on computer compatible magnetic tape.

The vertical wind velocity is calculated for each half second interval using the following basic routines:

$$W = W_{ac} - W_{meas}$$

Vertical wind equals vertical aircraft velocity minus aircraft velocity relative to the air.

$$W_{ac} = \int^t \dot{W}_{ac} dt \text{ with linear trend removed}$$

$$W_{meas} = TAS (\Theta - \alpha)$$

$$\alpha = \frac{11 \Delta P}{q} \quad \text{where } 11 \text{ is the wind tunnel determined empirical constant for the PSU gust probe}$$

$$q = \frac{\rho_{std} (IAS)^2}{2}$$

$$TAS = \sqrt{\frac{q}{2\rho}} \quad \text{where } \rho \text{ is the air density}$$

$$\rho = \frac{P}{RT}, \quad \rho_{std} = \frac{P_{STD}}{RT_{STD}}$$

Making all the necessary substitutions

$$W = IAS \sqrt{\frac{3.516T}{P}} \left(\frac{1795.7 \Delta P}{(IAS)^2} - \Theta \right) + \int^t \dot{W}_{ac} dt$$

where temperatures are specified in degrees Kelvin, pressures in millibars, velocities in meters per second, and angles in radians, respectively.

After the vertical velocities are computed, they are spectrally analyzed using the PSU SAFFT (Spectral Analysis Fast Fourier Transform) program. Figure 1 is an example of a ten minute run on a flight over St. Louis on August 17, 1973. It clearly shows that the wavelength (approximately scaled for the mean aircraft velocity) with the largest amount of energy is ≈ 105 meters. A large number of such analyses allows

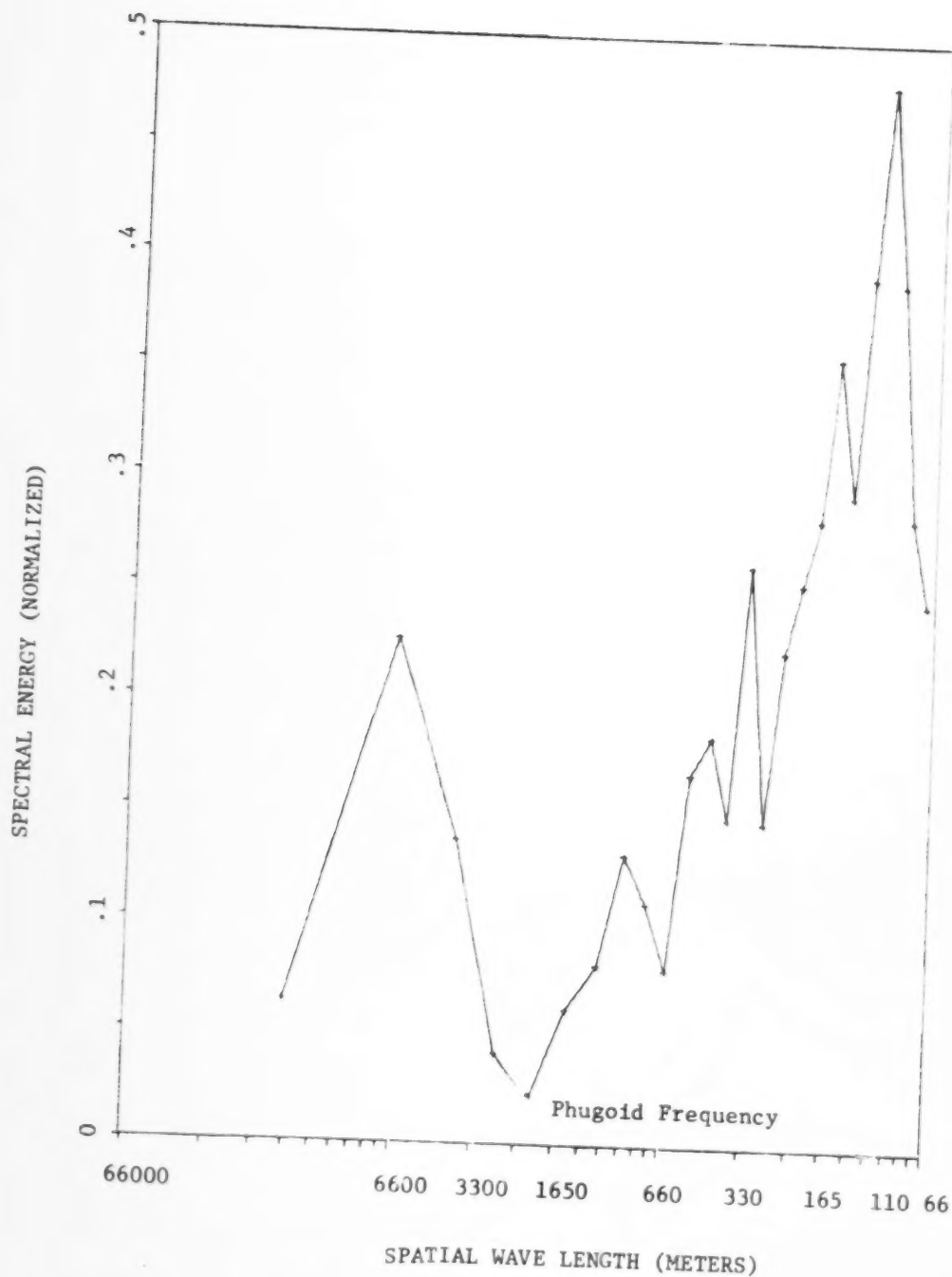


Figure 1. Spectrum of vertical velocity fluctuations recorded on 12 min run at ≈ 1300 AGL, 0830 CAT, 17 August 1973 over St. Louis, Mo.

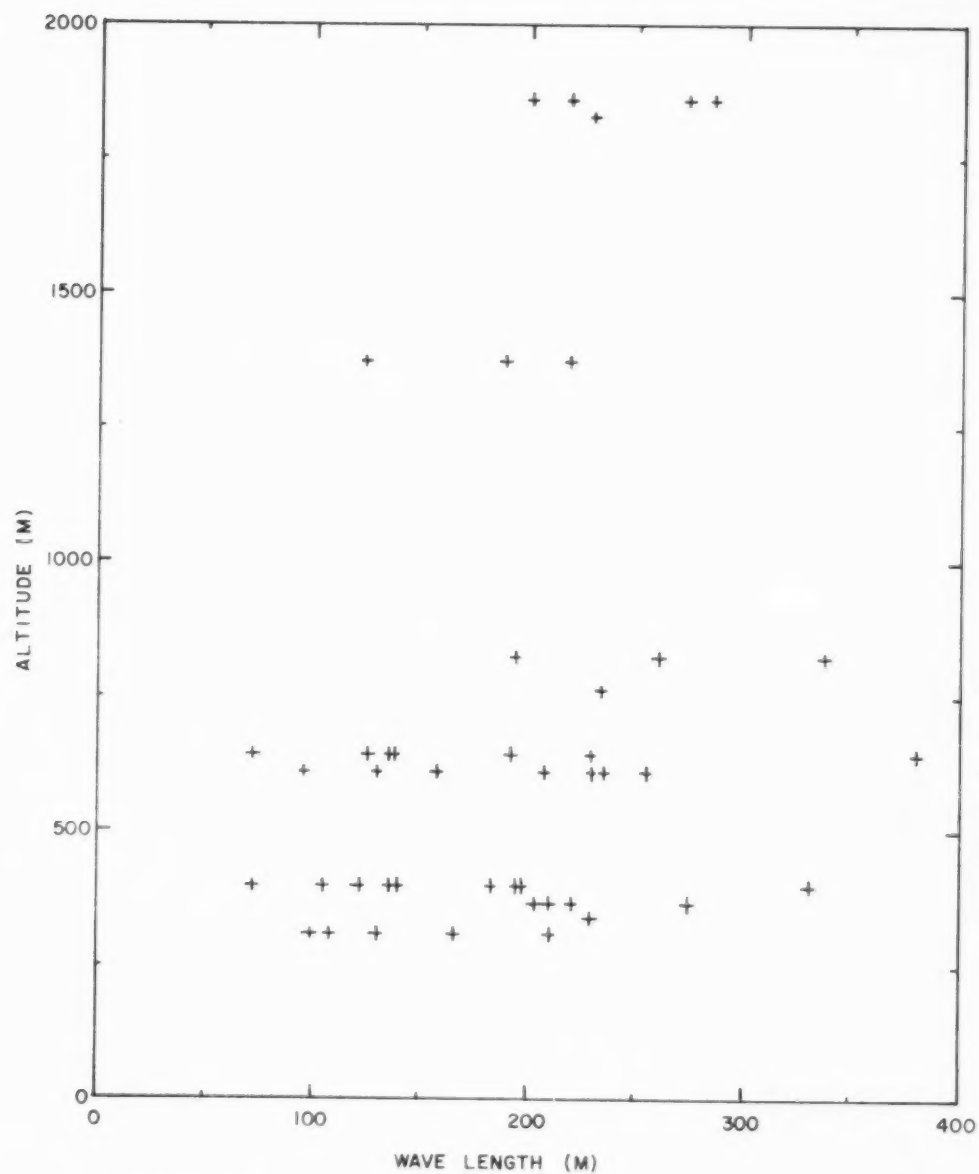
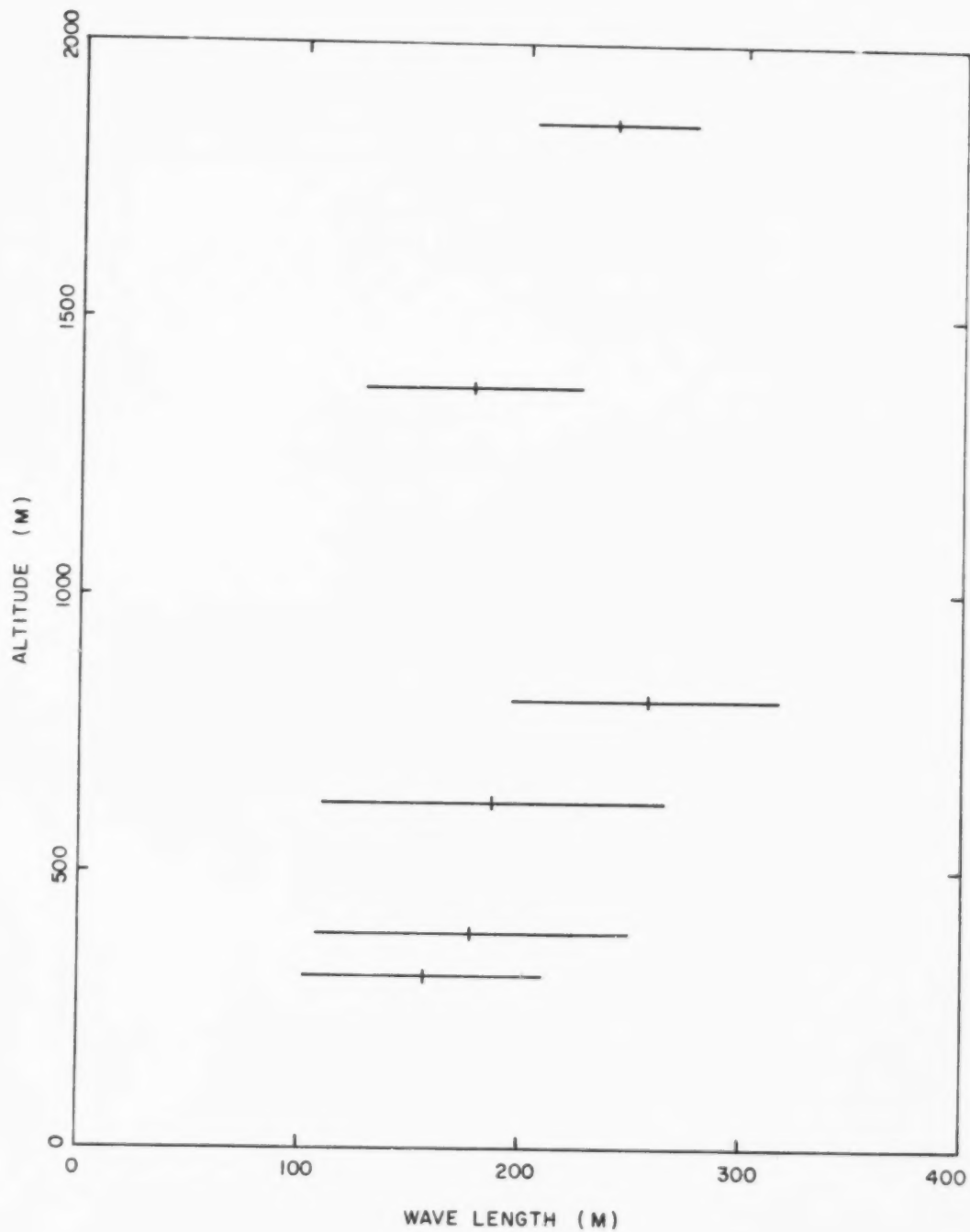


FIGURE 2 : CALCULATED WAVELENGTHS AS A FUNCTION OF ALTITUDE.



TURBULENCE ANALYSIS

FIGURE 3: ARITHMETIC AVERAGE
WAVELENGTH AS A FUNCTION OF ALTITUDE.
BARS DENOTE STANDARD DEVIATION.

us to plot the wavelengths or frequencies containing maximum energy against other factors such as altitude, surface roughness, or stability. Figure 2 is a scatter diagram of calculated wavelength versus altitude for 47 runs, all flown in August, 1973 on six different flights. Fig. 3 presents the arithmetic average wavelength as a function of altitude. Standard deviations of the means are also shown.

It should be noted that some observed data has been edited from our scatter diagrams. One occasional source of error is, for example, the aircraft's natural "phugoidal" period of oscillation, which is directly proportional to the air speed. It often appears in the spectral analysis during conditions with very light or essentially no turbulence. In these situations the phugoid will often have the largest amplitude on the spectral graph, but it obviously must be disregarded. Sometimes the dominant wavelengths in the analysis are larger than the altitude above the ground. In the turbulent planetary boundary layer, we assume that vertical wavelengths should be about the same as the horizontal and that the vertical should not normally exceed the altitudes at which they are measured. To date, these cases have not been included in the analysis.

Although processing of the individual turbulence runs is largely complete, analysis of the set of reduced data has only recently begun.

The distribution of turbulent wavelengths as measured by the aircraft does seem to be in general agreement with the theory proposed by Blackadar in an unpublished NASA report¹. The mixing length is given by

¹ Panofsky, H. A., 1972: Tower Micrometeorology. AMS Workshop on Micrometeorology.

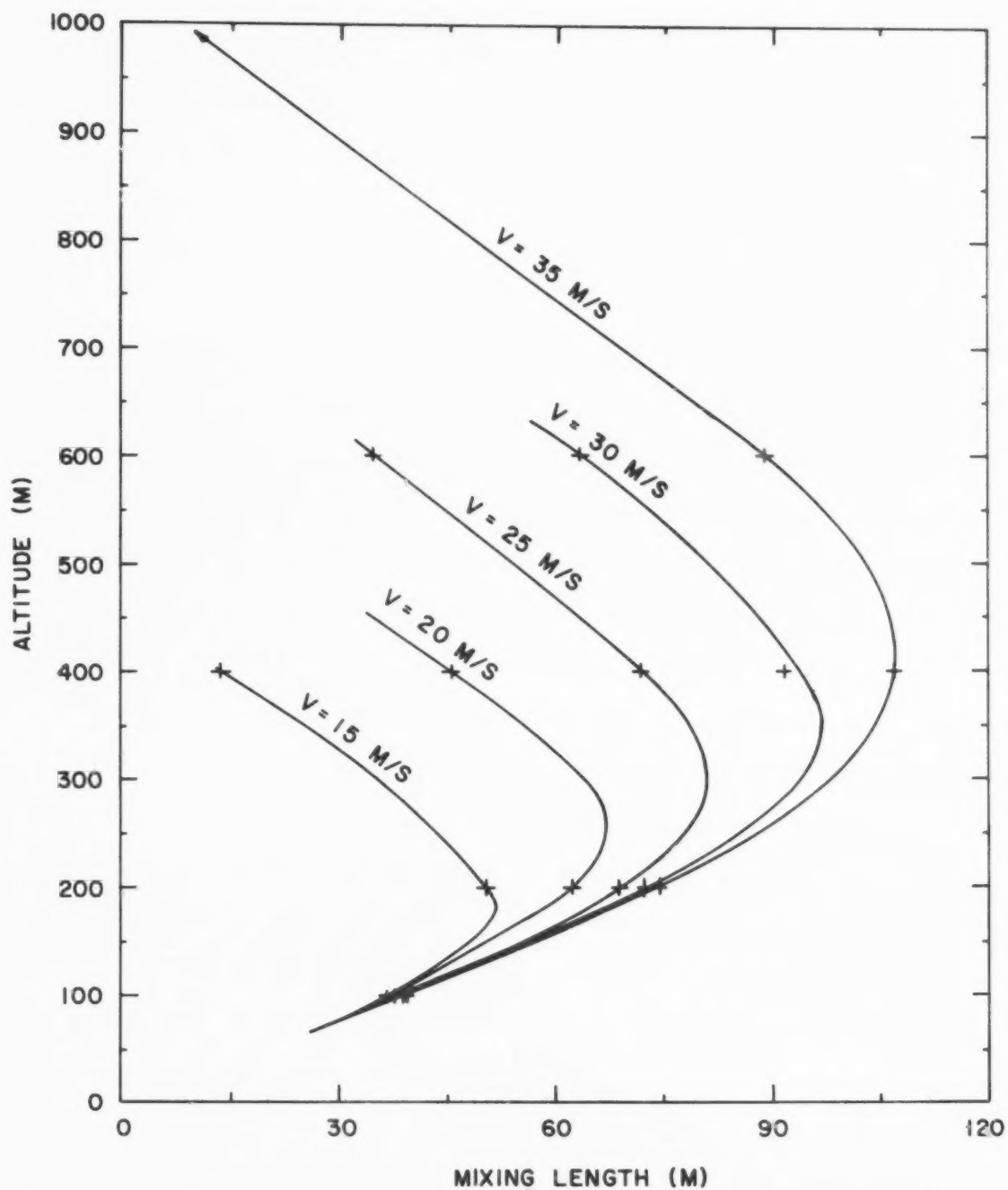


FIGURE 4. MIXING LENGTH VS. ALTITUDE AS PREDICTED BY BLACKADAR MODEL.

$$\ell = \frac{0.0063 u_{*0}}{f} \left(\frac{e^{\frac{kzf}{0.0063 u_{*0}}} - e^{-\frac{kzf}{0.0063 u_{*0}}}}{e^{\frac{kzf}{0.0063 u_{*0}}} + e^{-\frac{kzf}{0.0063 u_{*0}}}} \right)$$

$$u_{*0} = \frac{(V + 15 fz)k}{\ln \left(\frac{e^{\frac{fz}{0.0063 u_{*0}}} - e^{-\frac{fz}{0.0063 u_{*0}}}}{e^{\frac{fz_0}{0.0063 u_{*0}}} - e^{-\frac{fz_0}{0.0063 u_{*0}}}} \right)}$$

where ℓ = mixing length (m)

u_{*0} = surface friction velocity (m/s)

f = Coriolis parameter = 9×10^{-5} (sec^{-1}) at latitude 38°N

k = von Karman constant = 0.4

z = altitude (m)

V = wind velocity (m/s)

z_0 = roughness length = .5 (m) over the city

Neutral conditions and homogeneous terrain are assumed.

Figure 4 shows the relationship of mixing length to altitude for 5 different wind speeds. The curves were calculated and plotted using a programmable desk calculator. Since the aircraft data were gathered during a variety of stability conditions and over non-homogeneous terrain, it is not surprising that there is not better quantitative agreement with the

model. In particular, the slightly unstable average conditions combined with the large roughness length of the city compared to its surroundings have probably increased the depth of the planetary boundary layer to several times the predicted depth. Nevertheless, there is agreement to within an order of magnitude between predicted mixing lengths and observed turbulent wavelengths and, further, in the shape of the curves in that the larger values are observed in the middle altitudes. (Compare Figures 3 and 4.) Additional study is now underway to better establish the relationships between theory and the observations.

5.0 AIRBORNE MEASUREMENTS OF AEROSOL IN THE ST. LOUIS URBAN AREA

K. L. Schere

M. S. Thesis Research in Progress

Aerosol concentrations and the size spectrum of aerosols are expected to vary both as a function of distance from an urban complex and upon meteorological parameters. This research study consists of analysis of airborne aerosol measurements taken in and around the metropolitan St. Louis area during August, 1973, and July-August, 1974.

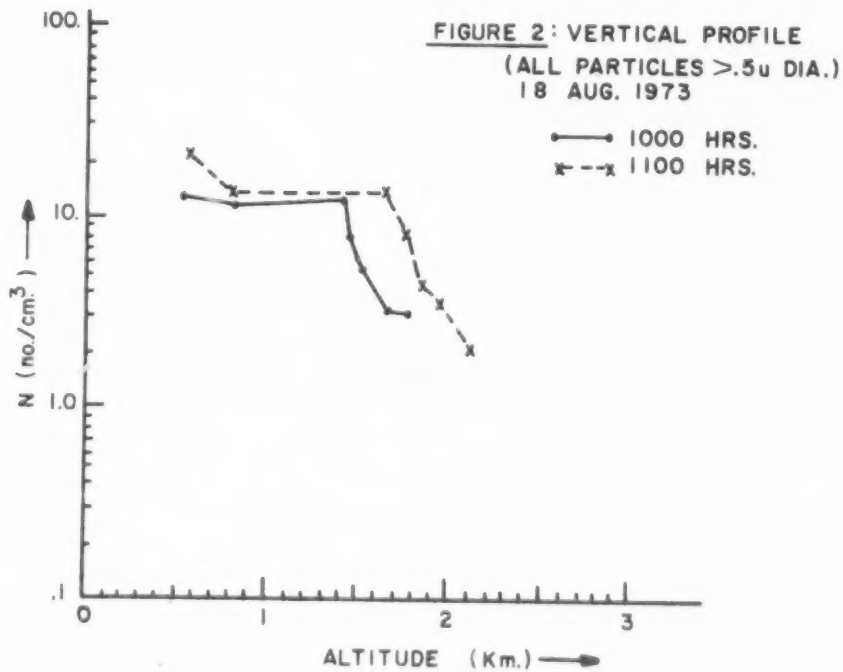
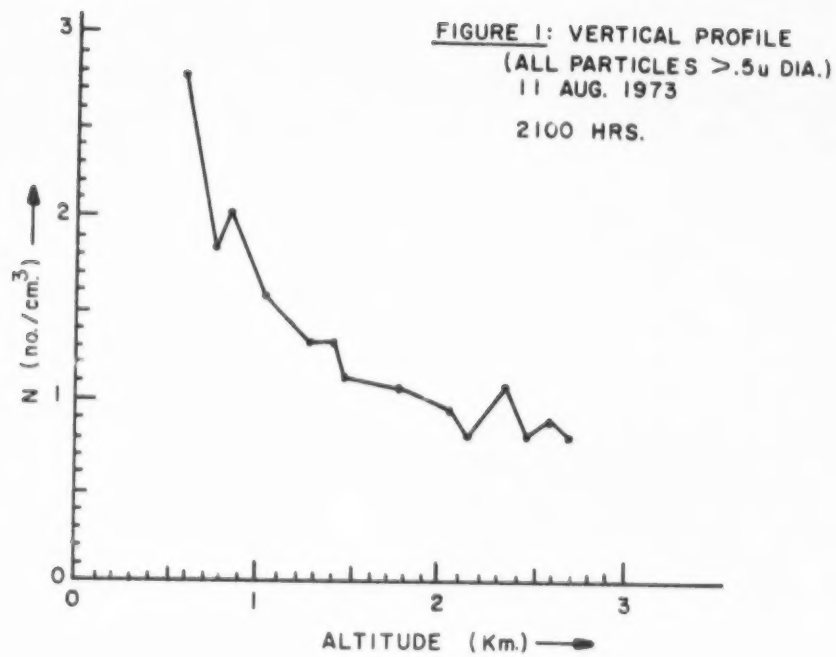
The instrument package on board the PSU Meteorology, twin-engine Aerocommander provides comprehensive meteorological, aerosol, turbulence and radiation measurements. The aerosol sampling instruments include a Royco particle counter #225, an M.R.I. Integrating Nephelometer, an Environment One-Model Rich 100 condensation nucleus counter, and a Thermo-Systems 3200A Mass Monitor. The Royco instrument has the capability of sampling small particles within discrete size ranges and can, thus, be used to measure in situ size distributions of aerosol particles within a range of about $.5\mu$ diameter to approximately 8μ diameter. The Integrating Nephelometer and the Mass Monitor provide indications of the total mass loading of small particles within the air. Although the two instruments utilize different physical principles in their operation, taken together they provide an adequate picture of the total particulate loading. The

Rich 100 instrument provides a count of the total number of condensation nuclei in the air, but the instrument cannot sample within discrete size ranges. Thus, in this study, the data from the Royco almost exclusively are used, while the data collected from the other aerosol sensors, although they provide perfectly good data sets by themselves, are being used only as reference or backup data. The isokinetic sampling probe, which is located on the top of the plane's fuselage so as to be adequately removed from the engine exhausts and skin venting, has been wind tunnel tested to verify that isokinetic flow exists at an air speed of 140 mph. This speed is maintained on all aerosol sampling flights in the Aero-commander.

Flight patterns used for measurements were of two types: (1) a vertical sampling pattern, and (2) a horizontal sampling pattern. The St. Louis area is assumed to be a 50 km diameter circle centered in northwest St. Louis city. The circle, thus, includes most of the major industries and the bulk of the population for the area. On any given flight day, the mean wind is then aligned through the center of this circle. For the vertical sampling pattern, four points are chosen on this line, over which samples are taken at altitudes ranging from 1500 feet msl ($\approx$ 1000 ft msl) to approximately 2000 feet above the height of the observed haze layer in steps of 1000 feet. The points are picked so that they are far upwind, near upwind, near downwind, and far downwind of the city. For the horizontal sampling pattern, six legs of varying length are flown normal to the mean wind line so that the entire St. Louis area is covered. The pattern extends 75 km downwind of center city and 50 km upwind. It is flown at one level within the haze layer and one level above it during the

afternoon hours. The vertical sampling pattern is flown three times during the same 24-hour period: Once in the morning hours around sunrise when the air is most stratified, once in the afternoon when the mixing is strongest, and once in the late evening when the inversion is just starting to form.

The data analyzed to date was collected during flights conducted in August, 1973. It appears that many non-source factors are influencing the distribution of particulates present in the air; including mean wind direction and speed, relative humidity, type of prevailing air mass, and time of day. From a previous study done in the St. Louis area, it was found that the mean mixing-depth for this time of year was about 1500 m. However, it was noted that afternoon mixing depths are often much higher than this. In order to more clearly see the vertical variation of total particulates ($> .5\mu$ dia.) plots were made from the data. It is found that during stable conditions, such as are prevalent at night, the atmosphere becomes stratified as a surface inversion frequently develops. When this happens, the total number of particulates gradually drops off with altitude until reaching a fairly constant background level. Figure 1 is such an illustration. This is the vertical profile of total particulates on August 11, 1973 between 2100-2200. The air mass over the St. Louis region at this time was a quite clean one as evidenced from the low particle counts. Figure 2 is a similar plot. Here the vertical profile is shown on August 18, 1973, at 1000 (solid line) and 1100 (dashed line). This plot illustrates two principles. First, during the daylight hours when the



mixing layer has been stirred well by convective currents, the homogeneity is very marked. There is a sharp drop-off of particle concentration above the mixed layer. Secondly, it is seen that the depth of the mixing layer increases as the convective heating from the earth increases. This is manifest by the displacement of the vertical profile to the right from 1000 to 1100 hours.

The size distribution of particles in the atmosphere was also estimated. The results are plotted using the same form as that used by Junge in his earlier work on this subject; that is $dN/d(\log r)$ vs. $\log r$. This scheme was chosen because the area under a plot of this type represents the number of particles. Junge found that for tropospheric aerosols the size distribution of particles greater than .1 μ dia. could be approximated by a power law of the form $dN/d(\log r) \sim r^{-3}$. In computing size distributions from the Royco particle counter data, a least-squares-fit technique was applied to the five points in each distribution. Since this is plotted on log-log axes a power-law results from each. It was found that in the mixed layer a typical plot was such as that shown in Fig. 3. A total of 19 particle size spectra were computed from the 1973 data, 18 of which were within the mixed-layer and only one of which was taken from data in the relatively clean air above the mixed layer. This distribution is shown in Figure 4. Note that the magnitude of the slope is less here and that the whole plot is displaced to a position beneath the one in Figure 3. This reflects the fact that the total particle loading is much smaller above the mixed layer and furthermore, that the decrease in number of the smaller

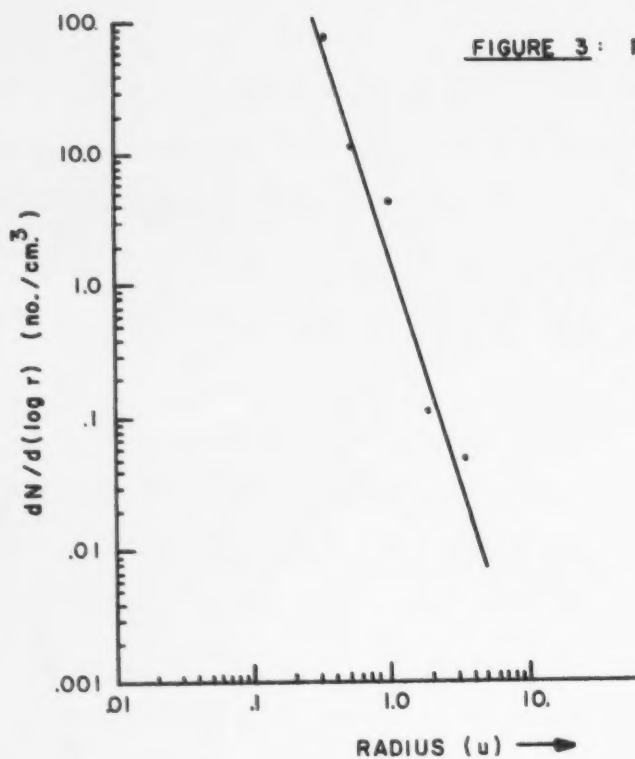


FIGURE 3: PARTICLE SIZE SPECTRUM

18 AUG. 1973

1000 HRS.

ALTITUDE = .56 KM.

$$dN/d(\log r) = 1.79 r^{-3.23}$$

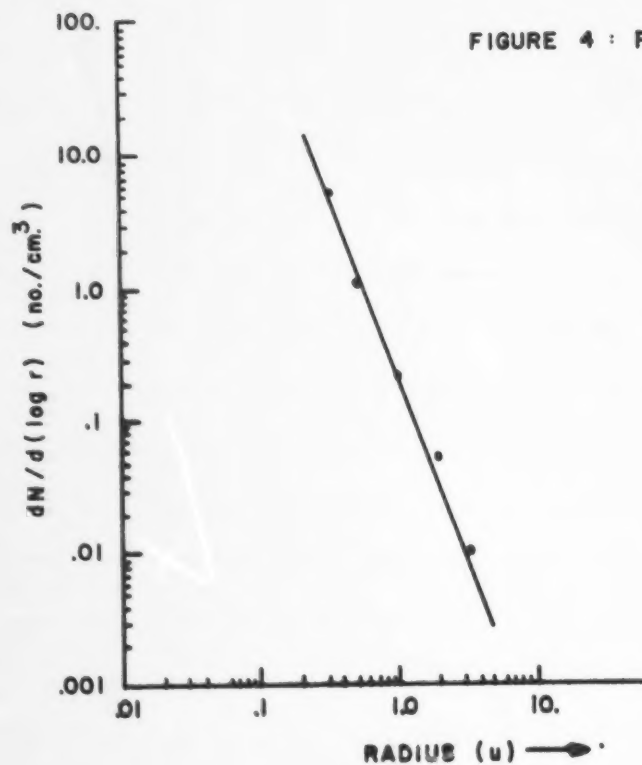


FIGURE 4: PARTICLE SIZE SPECTRUM

15 AUG. 1973

2000 HRS.

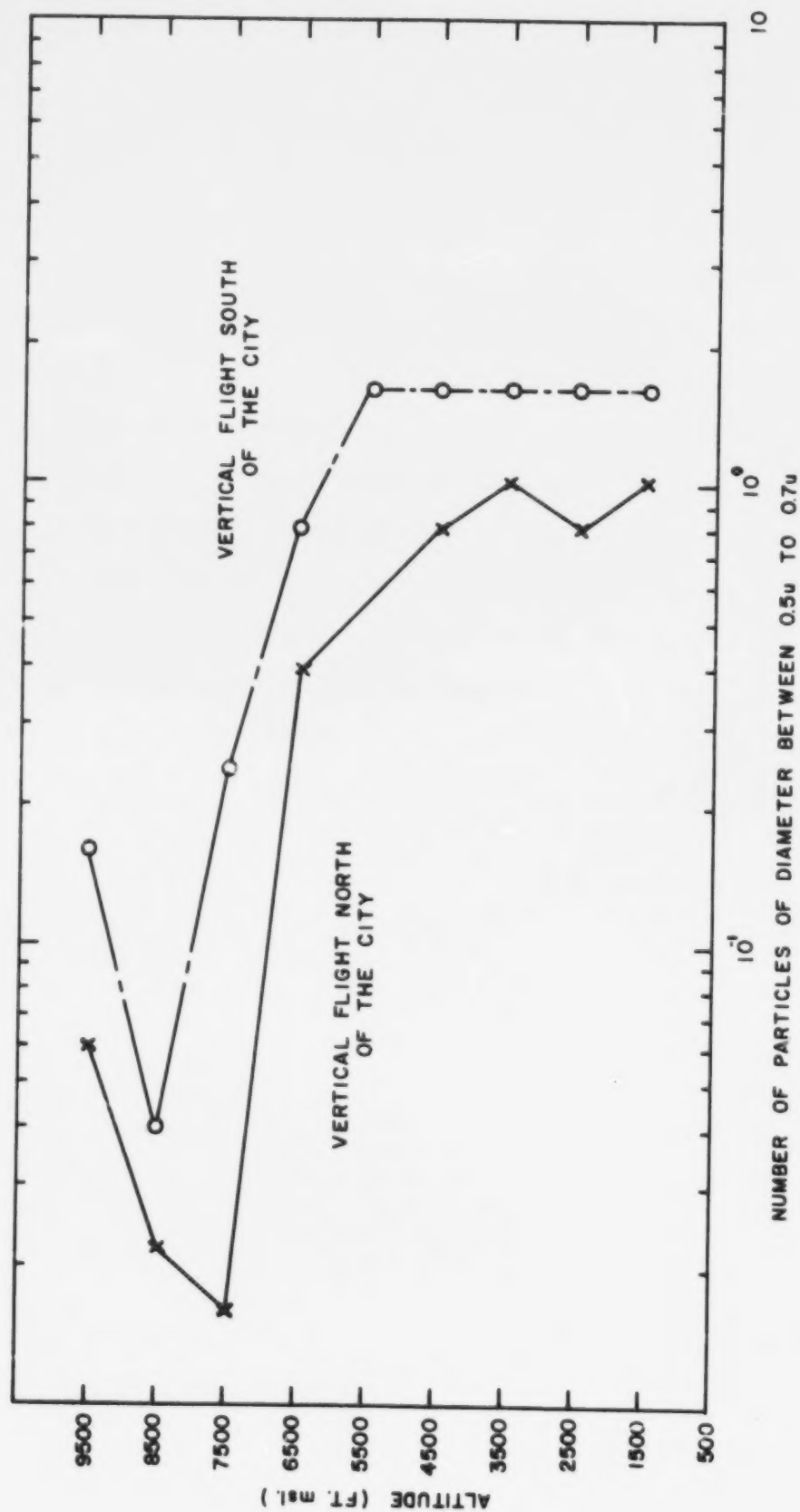
ALTITUDE = 2.65 KM.

$$dN/d(\log r) = 0.227 r^{-2.57}$$

particles is possibly more accentuated than the decrease of the larger particles here. Of course, more size distributions taken above the mixed layer are needed to establish this and thus, a special effort was made during the 1974 project to obtain these.

As this report was being written, preliminary analysis of the 1974 RAPS flight data was already underway. Figure 5, prepared by Y. Mamane, is an example of our most recent observations. Changes in the aerosol number concentration between the upwind (north) and downwind (south) sides of the city as well as the apparent structure of the planetary boundary layer are evident. These observations were extracted from the observer's log. Final "calibrated" results will not be available until the high resolution digitally-logged data is processed.

FIGURE 5 : VERTICAL PROFILE OF NUMBER CONCENTRATION OF PARTICLES OVER ST. LOUIS AREA ON AUGUST 5, 1974



6.0 SURFACE MEASUREMENTS OF AEROSOL IN A RURAL AREA USING DIFFERENT METHODS

Y. Mamane, Thesis Research in Progress

6.1 Introduction

The purposes of this project are to study in detail the characteristics of the suspended particulates in a rural area and to evaluate and intercompare different instruments, especially their indications of mass concentration, visibility and size distribution.

This report describes briefly one experiment, and summarizes and presents a preliminary analysis of selected data. Most of the data, recorded on magnetic tape, is to be processed during fall, 1974.

6.2 Instrumentation

In order to compare several "in situ" instruments, one must have a sampling system which causes negligible changes in the concentration and size distribution of the aerosol that is sampled. Furthermore, it must enable the instruments insofar as possible to simultaneously sense nearly the same sample of air. The sampling line shown in Figure 1 was designed and used for this study.

The sampling line has the following features. It:

- (a) is short,
- (b) has short horizontal sections,

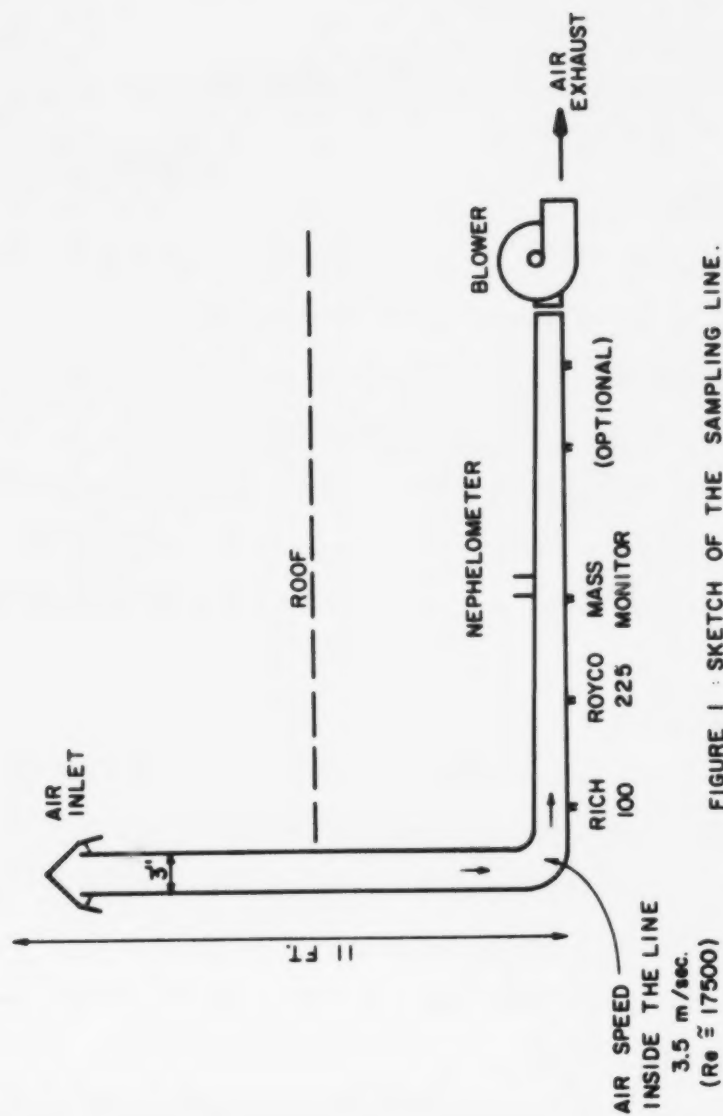


FIGURE 1 : SKETCH OF THE SAMPLING LINE.

- (c) is "smooth" with no change in cross section, and
- (d) is made of a large (diameter) pipe.

The instruments used continuously in this study were:

- (1) Integrating Nephelometer - MRI
- (2) Royco 225 Particle Analyzer
- (3) Mass Monitor, Thermo Systems 3200A
- (4) Rich 100 Condensation Nucleus Counter

Some other instruments such as a high volume sampler and cascade impactor were also occasionally used. Table I summarizes the characteristics of each instrument.

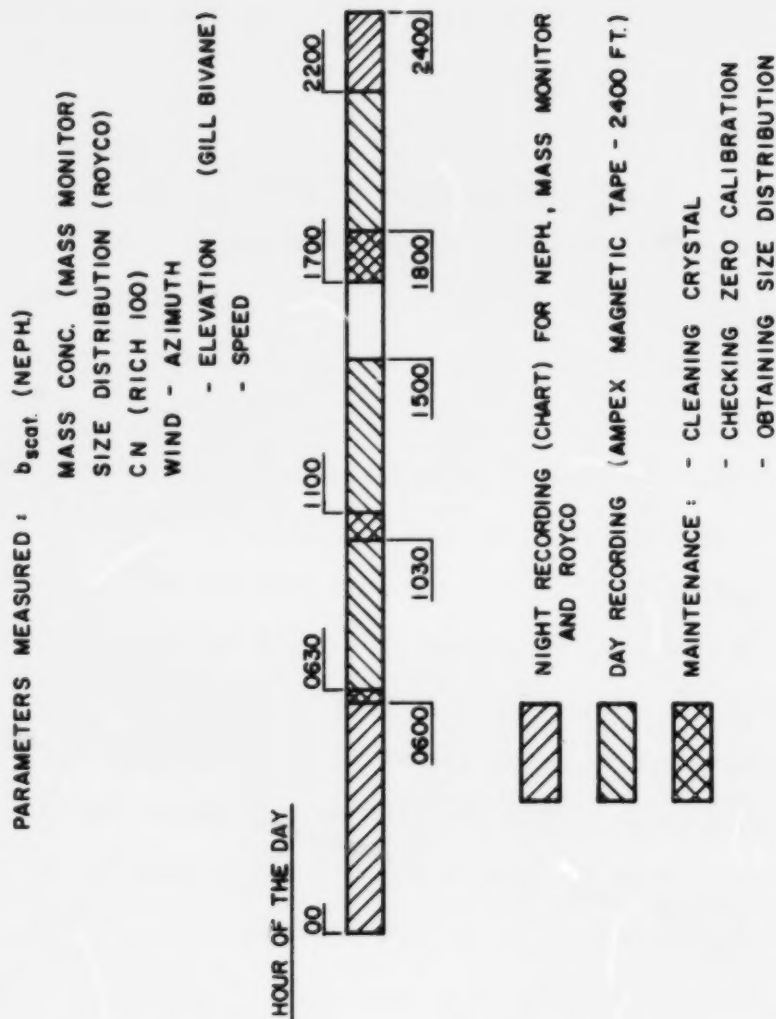
Instrument failures in the primitive field station and adverse weather conditions during the winter of 1973/74 made it difficult to obtain several days of continuous measurements from all the instruments.

The instruments were located in a cabin far from local sources of air pollution. At first, the instruments were run continuously, and the data was recorded on a strip chart (all the channels on the same chart). Beginning in summer (1974), the data was recorded on magnetic tape during the day and on a strip chart at night. This is described in Figure 2. The magnetic tape data has not yet been processed.

6.3 Summary of a Selected Data

Figure 3 summarizes data collected on March 5-6, 1974 by the Nephelometer and the Mass Monitor. There is fair correlation between the light scattering parameter and the mass concentration measured by the mass monitor. The factor which converts the light scattering to mass concentration,

FIGURE 2 - SUMMARY AND TYPICAL SCHEDULE FOR SURFACE MEASUREMENTS



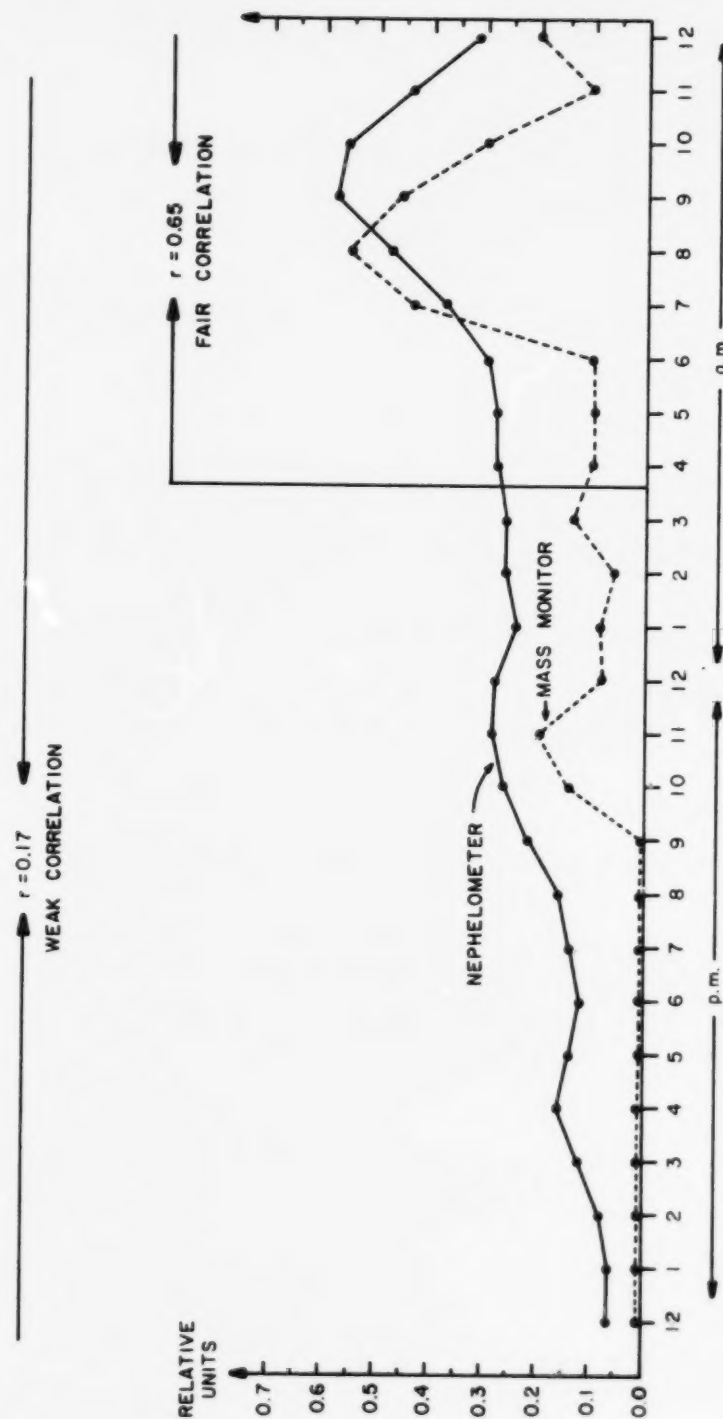


FIGURE 3 : COMPARISON BETWEEN THE NEPHELOMETER AND THE MASS MONITOR ON THE S-6 OF HARDI 1974.

Table 1
Instrumentation (aerosol)

	Mass Monitor	Nephelometer	Rich 100	Royco
Function	Concentration	Scattering Coefficient	Condensation Nuclei	Size Distribution
Particle Diameter	0.01 - 20 μ (probably not larger than 5-10 μ)	No limit	>0.0025 μ (probably not larger than 5-10 μ)	0.5 - 0.7 0.7 - 1.4 1.4 - 3.0 3.0 - 5.0 > 5.0 or 0.5-~10 μ
Flow Rate	1 ℓ pm	~800 ℓ pm	3 ℓ pm	0.27 - 2.7 ℓ pm
Signal Output	0 - 7.5 vdc	0 - 5 vdc	0 - 10 mv dc	0 - 0.1 v dc
Calibration	By Manufacturer	Freon-12	By Manufc.	By Manufc.
Maintenance	1) Cleaning Crystals	1) Electronic Calibration	1) Adding Distilled Water	1) Electronic Calibration
Warm-up	30 min.	30 min.	30 min.	Few min.
Response Time	Order of 1sec	$\approx$ 1 sec	~2 sec	$\approx$ 1 sec
Sampling Air Speed	~70 cm/sec (1/4"i.d.)	~900 cm/sec (1-3/4"i.d.)	~200 cm/sec (1/4"i.d.)	~200 cm/sec (1/4"i.d.)
Power Input		70 W	80 W	65 W

suggested by MRI, yields numbers which are more than five times higher than the results indicated by the mass monitor. A typical size distribution for that day is shown in Figure 4. This distribution is well represented by the model suggested by Junge:

$$\frac{dN}{dr} = ar^{-\beta}$$

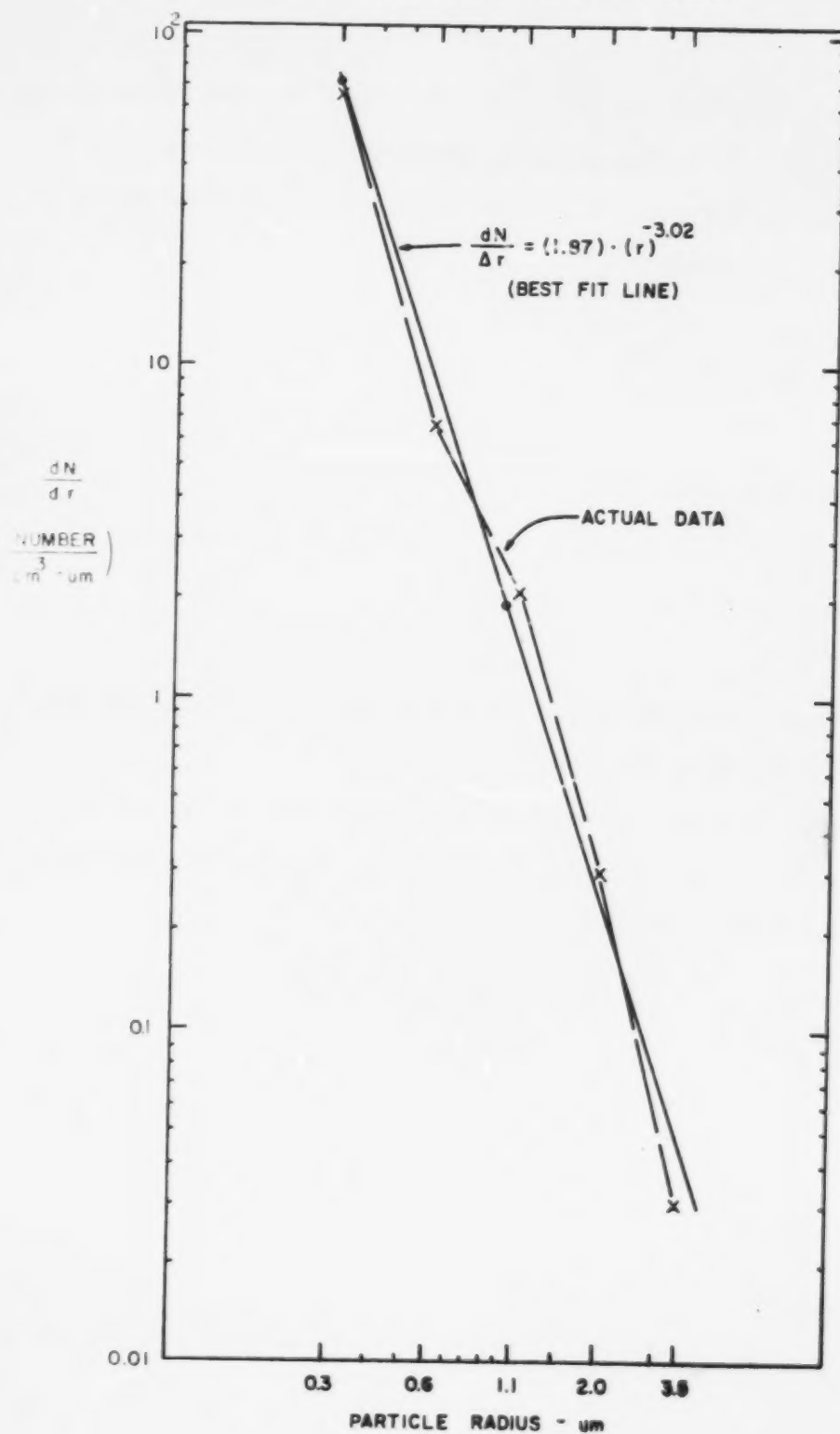
for this special case:

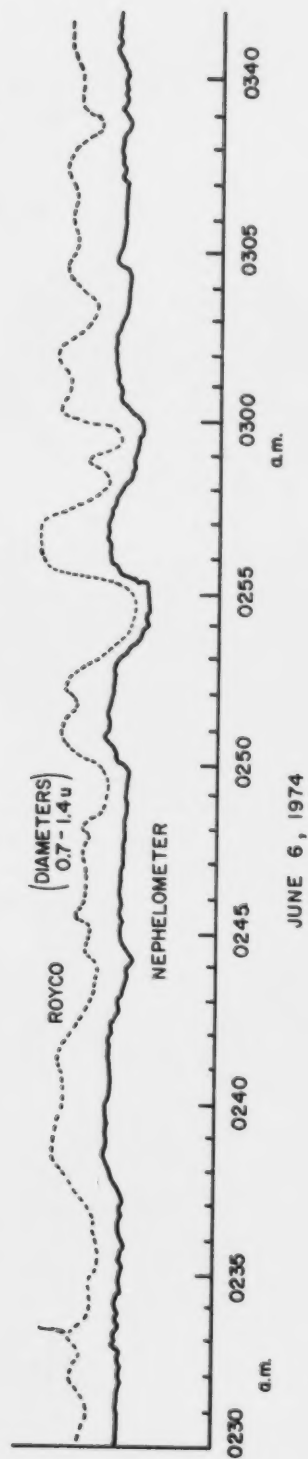
$$\frac{dN}{dr} = 1.87 r^{-3.02}.$$

Figures 5 and 6 show the highly correlated outputs of the Integrating Nephelometer and the Royco (for one class of sizes).

A meaningful comparison between the High Volume Sampler and the Mass Monitor is not yet available. Some data indicates that the mass monitor is underestimating total mass.

FIGURE 4: TYPICAL SIZE DISTRIBUTION ON MARCH 5, 1974





ROYCO		NEPHELOMETER	
AVERAGE	0.73 PARTICLES/cm ³	$1.4 \times 10^{-4} \text{ m}^{-1}$ (LIGHT SCATTERING)	
DATA POINTS	42	42	
STANDARD DEVIATION	0.11 P/cm ³	$0.14 \times 10^{-4} \text{ m}^{-1}$	

CORRELATION COEFFICIENT - 0.87

FIGURE 5: THE VARIATIONS OF THE NEPHELOMETER AND THE ROYCO DURING A SHORT TIME PERIOD.

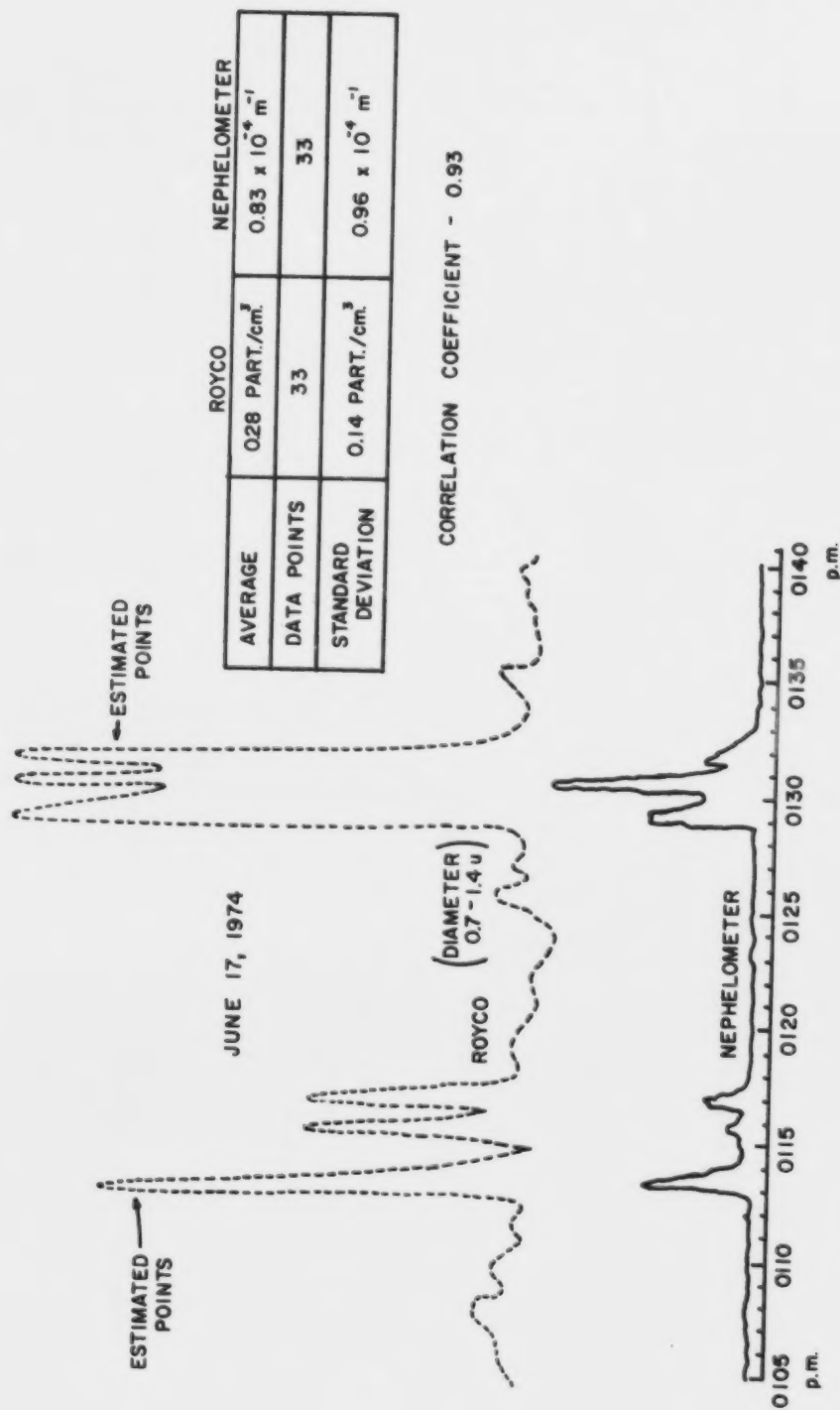


FIGURE 6 : THE VARIATIONS OF THE NEPHELOMETER AND THE ROYCO (0.7-1.4 u) DURING A SHORT PERIOD OF TIME.

7.0 TECHNIQUES FOR THE "MESOSCALE"

INTERPRETATION OF AIRCRAFT MEASUREMENTS

T. Chin, M.S. Thesis Research in Progress

Aircraft data can be used to precisely determine the state of the atmosphere on many scales as long as the time and space limits in which it was obtained are recognized. Clearly, the limits of validity also depend upon the method of data collection and the eventual use for which the data is required. The limitations, in both time and space, result from the basic nature of aircraft data. That is, it is asynchronous because a single aircraft flying at a finite speed can only sample a small atmospheric volume.

The aircraft data collected in conjunction with the SRG program consists, basically of two sets taken on an urban scale (2.5-25 km) and one on a mesoscale (25-250 km). The urban scale data was taken in the St. Louis area during the summers of 1973 and 1974. Each "urban" sampling run was on the order of ten minutes (36 km) long. The mesoscale data taken during October 16 and 17, 1974, within the boundaries defined by the SRG mesoscale model, consists of six flights of about 3-1/2 hours each, taken over the two day experiment period.

The ultimate utilization of each data set dictates the techniques which must be used in its reduction. Processing of the St. Louis data is, essentially, a problem of a categorizing and tabulating nature. The state of the atmosphere is measured and tabulated for various flight paths

at various times and altitudes over the St. Louis area. The time intervals of the sampling runs are short compared to the time scale of the large scale phenomena under study, such as changes in stability and changes in the concentration and distribution of aerosol. In this case, then, the problem of asynchronous data is relatively unimportant. Each sampling run may be treated as if all the data points were obtained simultaneously.

Because the SRG group had accumulated experience in processing turbulence data, its processing presented no serious problems. However, corresponding aerosol measurements were plotted and found to have a much larger high frequency content than anticipated. To aid in visual inspection of the data, we decided to digitally filter it and, thus, remove most of the high frequency fluctuations. Initially, a seven point "Martin-Graham" filter with a cutoff frequency of 0.1 hz and termination frequency of 0.6 hz was tried. (The aircraft sampling frequency was 2.0 hz.) Due to the nature of the filter, it did not adequately attenuate the high frequency components. This is because the response function of such a filter is not zero beyond the termination frequency, but in fact, increases in the negative direction until it becomes - 0.2 at 1.0 hz. A second disadvantage of a filter with such a response function (with changing signs) is that there will be phase shifts in any Fourier analyzed data. To eliminate these undesirable features, the data was filtered by a seven point binomial filter, whose response function is always positive and effectively zero beyond 0.7 Hz. Figure 1 compares the response functions of the two filters. It appears that although the Martin-Graham type digital filters

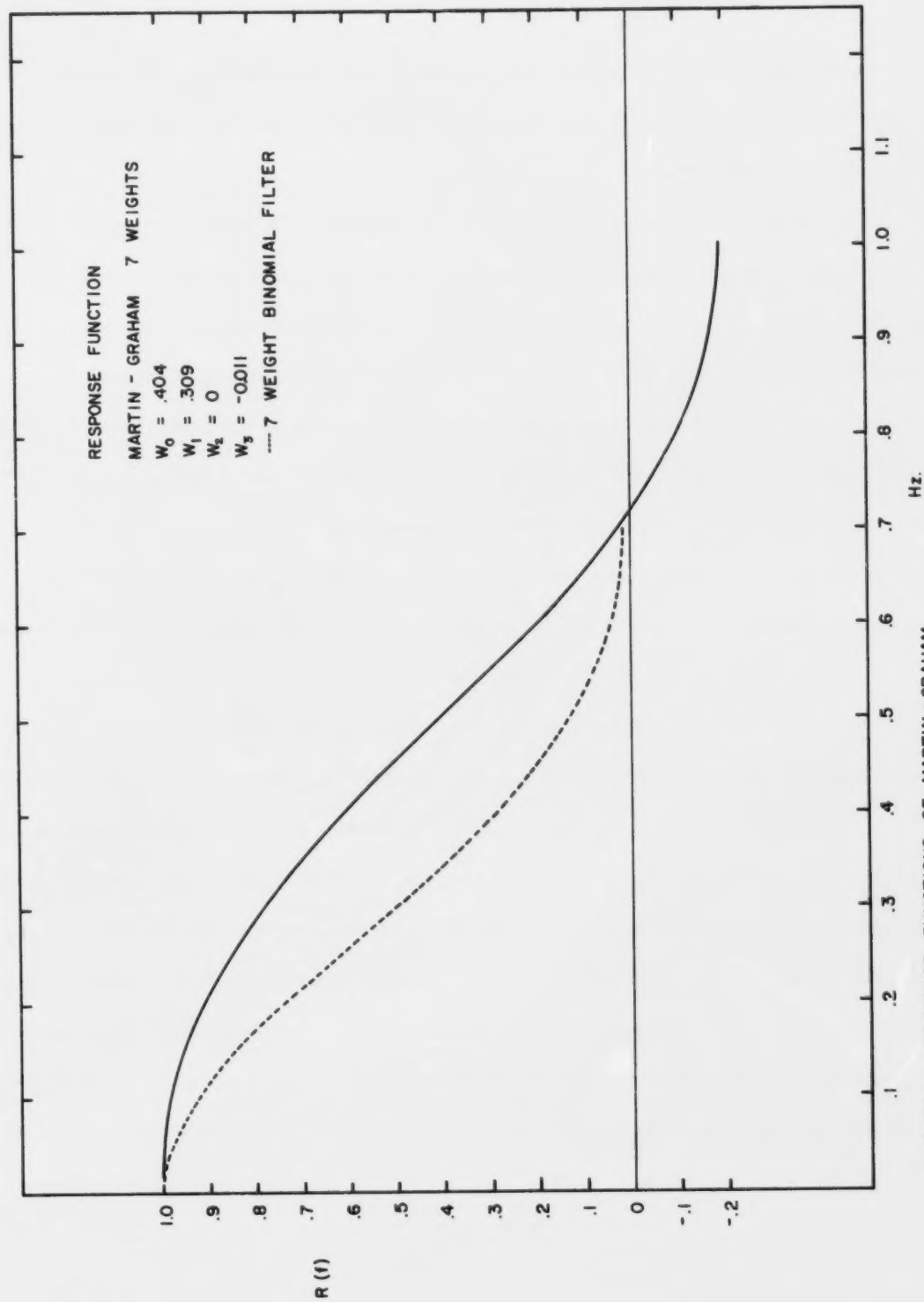


FIGURE 1 : RESPONSE FUNCTIONS OF MARTIN - GRAHAM AND BINOMIAL FILTERS.

can be designed with extremely sharp cutoff characteristics, for most urban-scale aircraft data interpretation problems, the binomial filter has better properties.

The mesoscale data is being used, in conjunction with other data sources such as radiosondes and surface observations, for initialization and verification at the mesoscale model. In this experiment, an entire sampling run took two days to complete. Each day's data collection consisted of flying over the same ground tract in a series of three flights (see Fig. 2). Each flight leg required a flight of about 3-1/2 hours duration. Refueling stops were made between legs. Thus, the time scale of the phenomena under study, evaluation of the mesoscale features of the atmospheric flow, was of the same order as the total sampling interval. The asynchronous nature of the data must, thus, be taken into account.

Firstly, to facilitate the use of this data for initialization and/or verification purposes, a pressure normalization program was written. Given a representative sounding, i.e., the distribution of temperature, dew point temperature, wind speed, and wind direction with pressure, the same variables as measured by the aircraft are reduced or normalized to any desired pressure level. As the program is now used, the atmosphere is assumed to be in a steady state condition and the gradients of the above variables to be horizontally homogeneous. These conditions are imposed because to date only one sounding has been utilized for normalizing the data collected during an

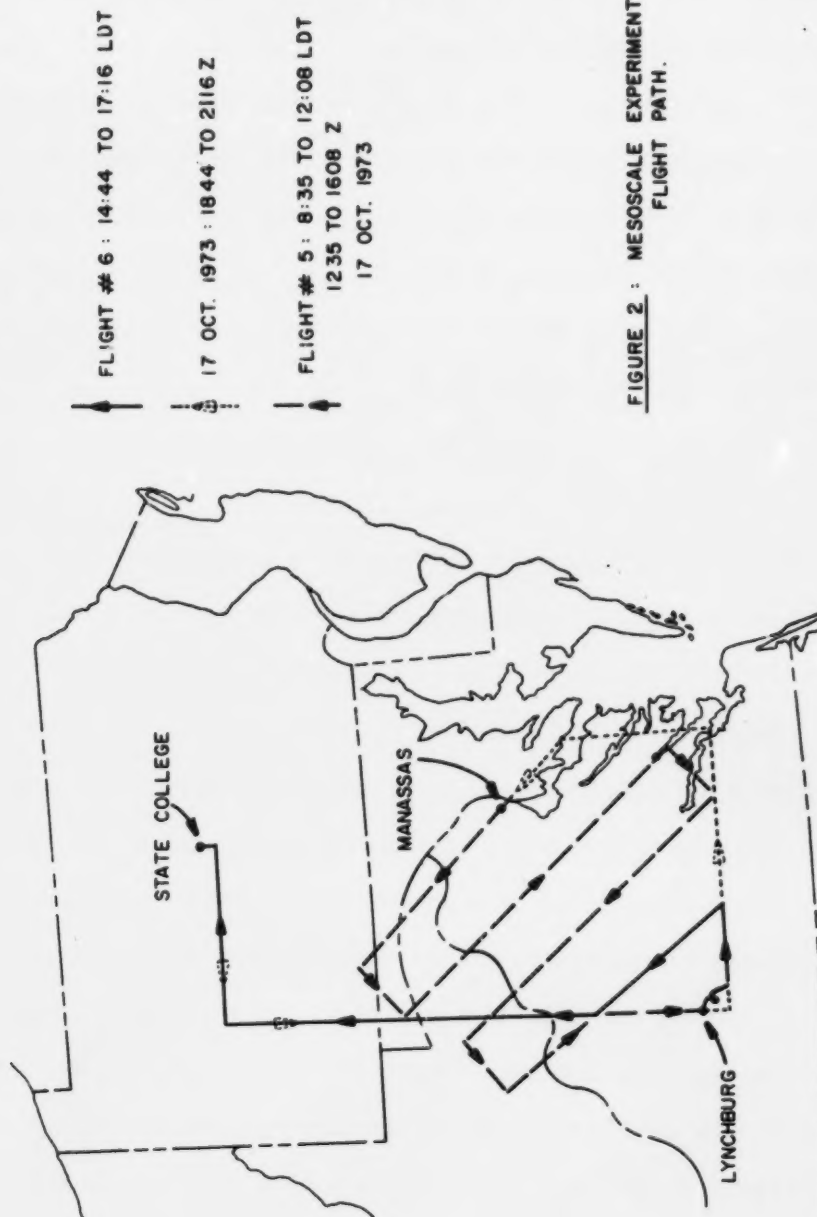


FIGURE 2 : MESOSCALE EXPERIMENT
FLIGHT PATH.

$\approx$ 12 hour period. The main purpose of this program is to, of course, provide a means for generating values for the temperature field, the moisture field, and the wind fields at any pressure level in the domain covered by the aircraft. Since the aircraft flies the ground track at various altitudes, it is normally difficult to separate vertical from horizontal variations. Analysis to date indicates that the normalized data does reflect much more clearly the horizontal gradients in temperature moisture and wind speed and direction.

Figure 3 illustrates the effects of pressure normalization on flight pressure and temperature traces, respectively.

The straight forward pressure normalization program described above represents, clearly, only a first step at best, and it does stretch the limits of validity of the data. Nevertheless, it is, even in its present form, still useful. For the conditions on October 16 and 17, the mesoscale model predicted a warm surface low in the southeasternmost region of the model domain. The warm region was barely discernable in the unnormalized plots of the temperature field, but clearly evident in the normalized plots.

A two dimensional plotting program has also been written. It divides the region of aircraft coverage into a grid in which the grid lengths are 4 to 5 times smaller than the grid lengths of the mesoscale model. Using the normalized data and calculating the position of the aircraft ground track with respect to this new grid, all data occurring inside a single grid interval are simply averaged. In this way an averaged, spatial picture is obtained for the pressure level to which the data was normalized. Fitting

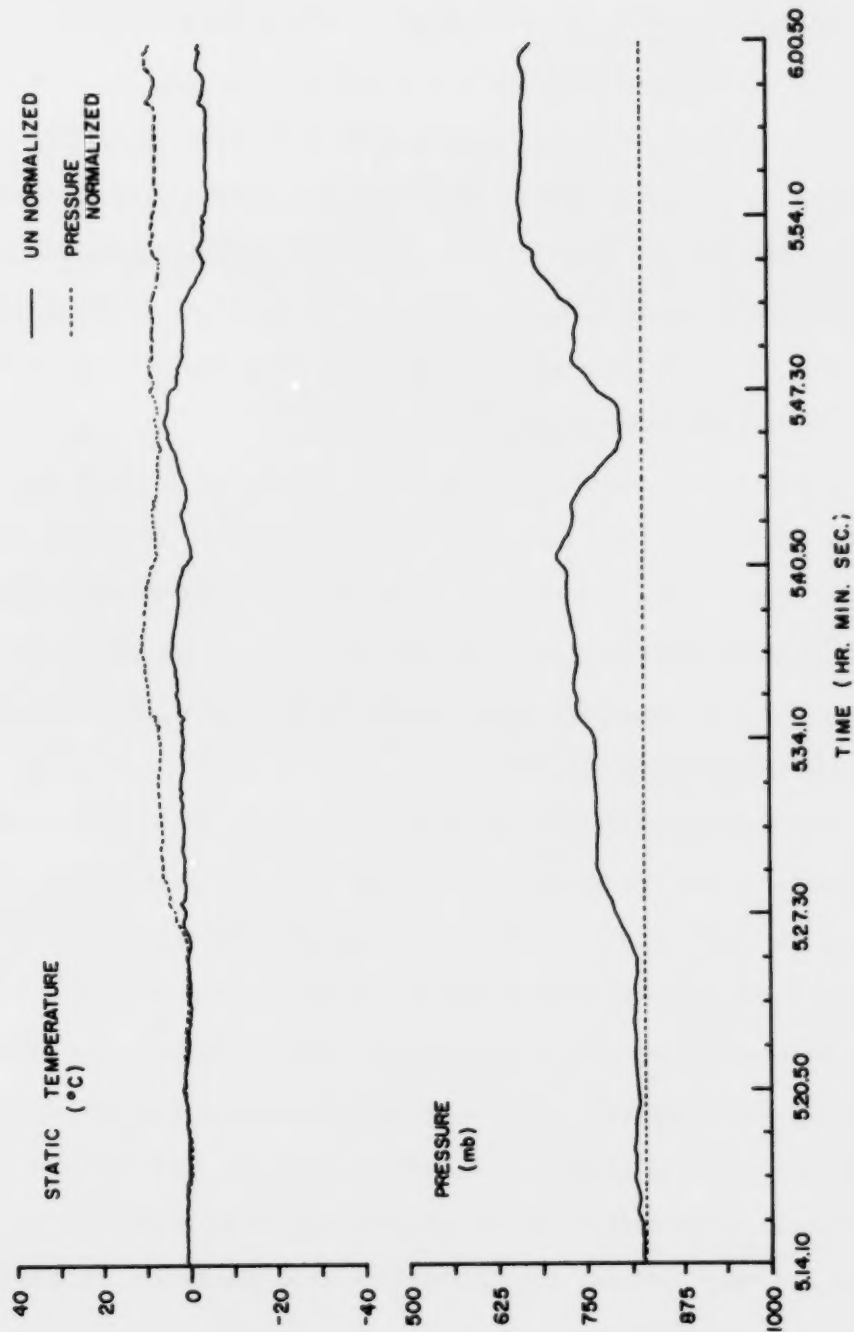


FIGURE 3 : SAMPLE PLOT OF UN NORMALIZED AND PRESSURE NORMALIZED DATA.

and interpolation schemes are being added to this program to fill in neighboring grid points through which the aircraft did not fly. By combining this program with the pressure normalization program for various pressure levels, a three dimensional description of the various parameter fields can be obtained. Once the three dimensional array is generated, it is a simple matter to generate any vertical cross section of the region or to generate any surfaces (at levels appropriate in the model) of the fields under study.

Modifications are underway to include a scheme for updating the sounding information used in the pressure normalization program. This will remove the present steady state restriction. The desirability of removing the horizontal homogeneity restriction in the gradients of the fields is low at this time. A numerical model should be initialized and verified against observed not computed data.

The asynchronous nature of the data can be dealt with, especially when the data is used for verification. The times at which the aircraft passes over the grid points in the mesoscale model are known. The model is simply instructed to output its predicted values for the fields at the times the aircraft flies over a grid point. The predicted value at that grid point is then compared to the averaged pressure normalized aircraft values, at any pressure level. In a similar fashion, this data can be used in the initialization made by first starting the model with balanced large scale data and then updating the appropriate grid points at the correct times.

VI OTHER CONTRIBUTIONS

Part 1

A GENERAL APPROACH TO DIFFUSION FROM CONTINUOUS SOURCES

R. Draxler

H. Panofsky

1.0 A GENERAL APPROACH TO DIFFUSION FROM CONTINUOUS SOURCES

R. Draxler and H. Panofsky, Research in Progress

1.1 Theory

There exist many methods for estimating dispersion from continuous point sources. In this project, an effort is made to bring together experimental data from many field studies in order to formulate a useful generalized treatment.

We begin with Taylor's diffusion theorem in Pasquill's form for lateral and vertical dispersion respectively:

$$Y(t) \equiv \frac{\sigma_y}{\sigma_v t} = \sqrt{\int_0^\infty F_v(n) \left(\frac{\sin \pi n t}{\pi n t}\right)^2 dn} \quad (1)$$

and

$$Z(t) \equiv \frac{\sigma_z}{\sigma_w t} = \sqrt{\int_0^\infty F_w(n) \left(\frac{\sin \pi n t}{\pi n t}\right)^2 dn} \quad (2)$$

Here σ_y and σ_z are the standard deviation of the mass distribution in the lateral and vertical directions, σ_v and σ_w the standard deviations of the lateral and vertical wind components. The diffusion time is t and is approximated by x , the travel distance, divided by mean wind speed. Hence $Y(t)$ and $Z(t)$ can alternatively be defined by

$$T(t) = \frac{\sigma_y}{\sigma_A x}, \quad Z(t) = \frac{\sigma_z}{\sigma_E x} \quad (3)$$

In these expressions, x is mean downstream distance, $F(n)$ denotes normalized Lagrangian operator of velocity components shown by the subscript and n is Lagrangian frequency; σ_A and σ_E are standard derivations of azimuth and elevation angle.

The quantities $Y(t) = Y(x/V)$ and $Z(t) = Z(x/V)$ are often expressed by power laws. However, in contradiction to power laws, both these quantities approach unity for small x . We have attempted to remove this inconsistency.

In order to evaluate the behavior of $Y(t)$ and $Z(t)$, we assume that, as for Eulerian spectra, we may write:

$$nF_v(n) = \phi_v \left(\frac{t}{T_v} \right)$$

and

(4)

$$nF_w(n) = \phi_w \left(\frac{t}{T_w} \right)$$

where ϕ_v and ϕ_w depend only on Richardson number, and T_v and T_w are proportional to the Lagrangian of turbulence for v and w . Eq. (1) then leads to the conclusion that $Y(t)$ and $Z(t)$ depend only on t/T_v or t/T_w , and Richardson number or z/L . We define T_v and T_w here such that $Y(t - T_v) = Z(t - T_w) = 1/2$.

For practical diffusion estimates, T_v and T_w have to be estimated first; then, eq. (1) gives $Y(t)$ and $Z(t)$ from which σ_y and σ_z can be calculated given σ_A and σ_E .

The method is most likely to be useful for estimates of σ_y , because the assumption underlying Taylor's diffusion law are best satisfied in the lateral direction.

1.2 Analysis

In practice, lateral and vertical dispersion from ground and elevated sources are analyzed separately, giving a total of 4 categories. There is some hope that lateral dispersion from ground and elevation sources behave in about the same manner except in very stable conditions.

At the time of writing of this report, only lateral dispersion from ground sources has been analyzed completely.

Figures (1) and (2) show the quantities Y plotted as function of T/T_v for 5 field experiments with ground releases for day and night. The same function appears to fit both figures about equally well. An approximate fit is provided by:

$$Y = \frac{1}{1 + 1.022 \left(\frac{t}{T_0}\right)^{0.595}} \quad (5)$$

except that the actual decrease at large σ/T_1 is somewhat slower than that indicated by the equations.

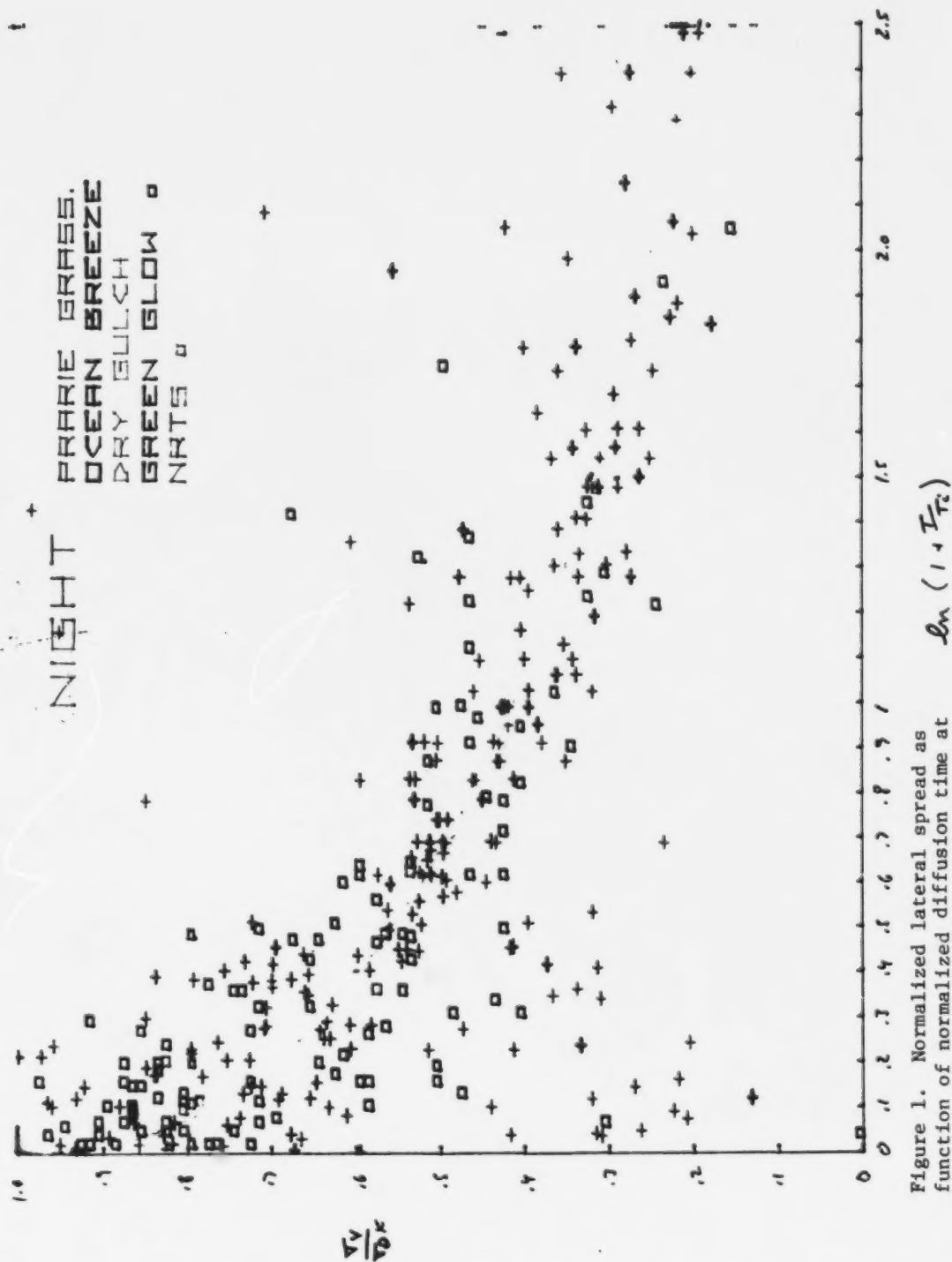
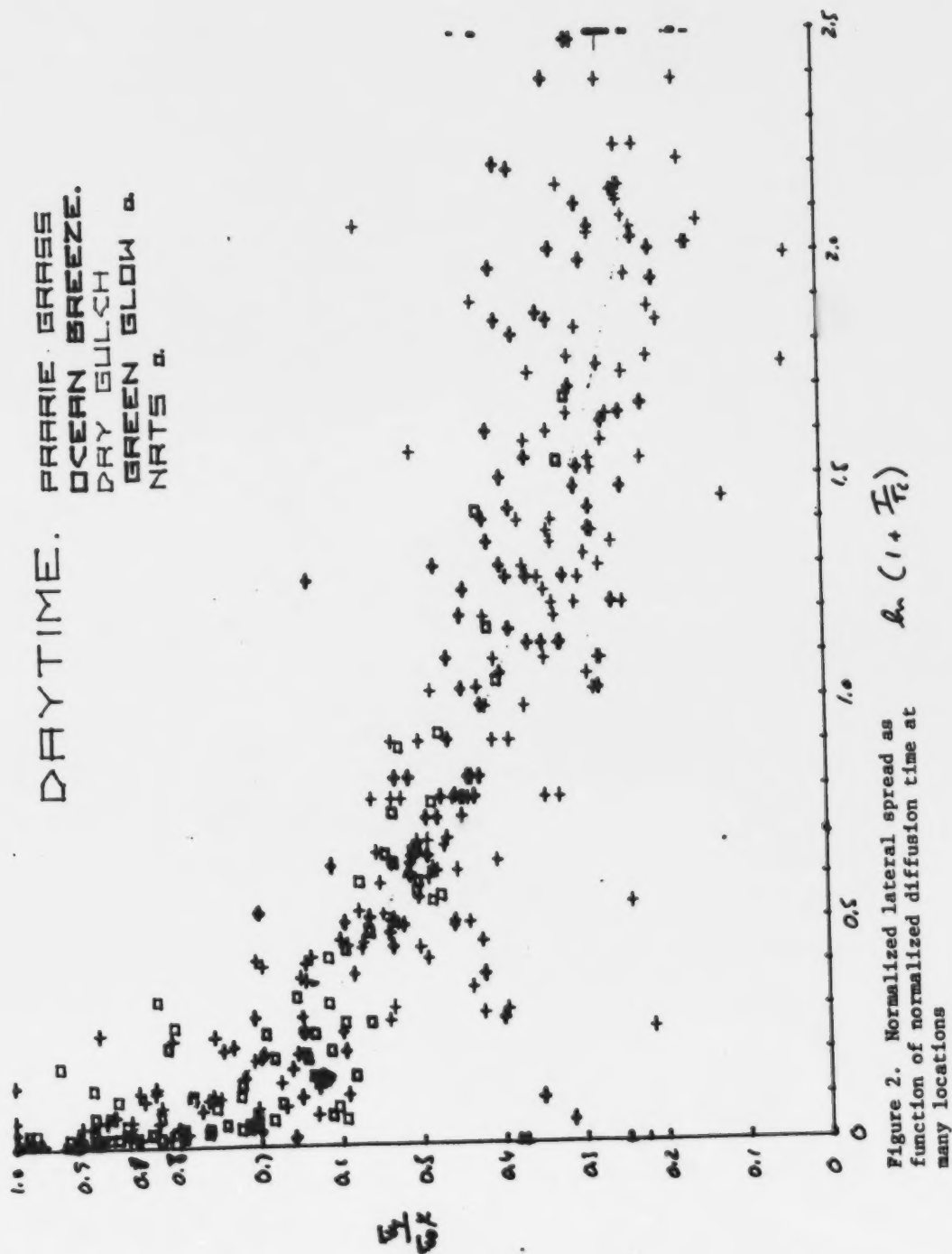


Figure 1. Normalized lateral spread as function of normalized diffusion time at many locations



The Lagrangian scale T depends upon the Richardson number but only weakly, in the sense that T_v is largest in unstable air. Unfortunately, the results from Hanford (Greenglow) give systematically larger T_v 's than expected from elsewhere. The reason for this discrepancy is not yet known to the authors. However, if we disregard this anomaly, we can obtain T_v from Ri ; hence, equation (5) gives Y , which yields σ_y if σ_A is known.

A similar analysis for vertical spreading from ground sources is in progress and appears less successful. There are only a few usable experiments and, so far they have yielded inconsistent results. One difficulty may be that this category least obeys the assumptions (such as homogeneity) underlying Taylor's theory.

Elevated sources look promising, but analysis is just beginning

VI OTHER CONTRIBUTIONS

Part 2

THE NIGHT-TIME MIXING DEPTH AT PHILADELPHIA

R. Hall

H. Panofsky

2.0 THE NIGHT-TIME MIXING DEPTH AT PHILADELPHIA

R. Hall and H. Panofsky, Research in Progress

2.1 Introduction

In cities, night-time pollution concentrations are commonly higher than day-time concentrations; in part due to the low wind speed, and, in part due to the small mixing depth. Both must be estimated from relatively limited information.

It has become customary to estimate night-time depth using a rural sounding by adding a 3°C increment to the surface temperature and drawing an adiabat to the sounding. Clearly, such mixing depths are unsatisfactory, for they imply that the "heat-island" effect of the city is always 3°C . We know from many models of the heat island that the temperature increment is quite variable depending on heat input, wind speed and the initial lapse rate. We have attempted to compare actual mixing depths with 3°C mixing depth (denoted here by h_{+3}).

Ideally, two soundings are needed for such a test; an upwind rural sounding, and a sounding just downwind of the city. Lacking such data, observations were obtained from Philadelphia where one sounding is made every morning near sunrise to the south of the city. With north winds, the city's heat island should be evident; even with south winds, there ought to be a heat island (perhaps smaller) due to an industrial complex situated to the south of the radiosonde launch site.

2.2 Analysis of observations

Winds and temperature sounds were selected according to the following criteria: wind direction between 315° and 45°, or between 135° and 225°; unstable or near-neutral large rates in the lower levels; mixing depth less than 400 m; low-cloud cover less than 3/10 and/or high clouds less than 7/10 at 10,000 ft or above. Also h_{+3} was recorded as estimated by National Weather Service personnel.

The observed mixing depths were subjected to various types of regression analysis, guided by Summer's formula which states

$$h = \sqrt{\frac{2H_x}{\bar{u} \alpha \rho c_p}} \quad (1)$$

where H is the heat flux, $\bar{u}$ the mean wind speed, x the fetch over the city, α the difference between rural and city lapse rates, ρ the density and c_p the specific heat at constant pressure. The rural lapse rate was assumed to be the lapse rate above the mixed layer.

2.3 Results

The winter mixing depths for north winds were generally high in accordance with the fact that pollution problems rarely arise under such conditions. This is probably because the lower atmosphere is

well-mixed before it reaches the city, due to heating from below.

The additional heating by the city sometimes shows up as a slightly more unstable lapse rate in the lowest few hundred meters.

This "incremental" heat island effect was small and not significantly related to any of the available predictions. It is probably of little operational importance, as the mixing depth is already high before the air reaches the city.

Summer mixing depths are consistently lower than in winter. They were analyzed in terms of wind speed and direction. In contrast to the predictions of eq. (1), the mixing depth appears to increase slightly with increasing wind, suggesting that the heat flux may be greater on windy than on calm nights. The effect of wind on lapse rate did not explain the result.

The best relation appeared between measured mixing depth and h_{+3} , (Fig. 1) where

$$h = 0.6 h_{+3}$$

suggesting that h_{+3} overestimates the mixing depth significantly and underestimates the pollution potential severely. Of course, this result is valid for Philadelphia only, and analogous studies should be made elsewhere.

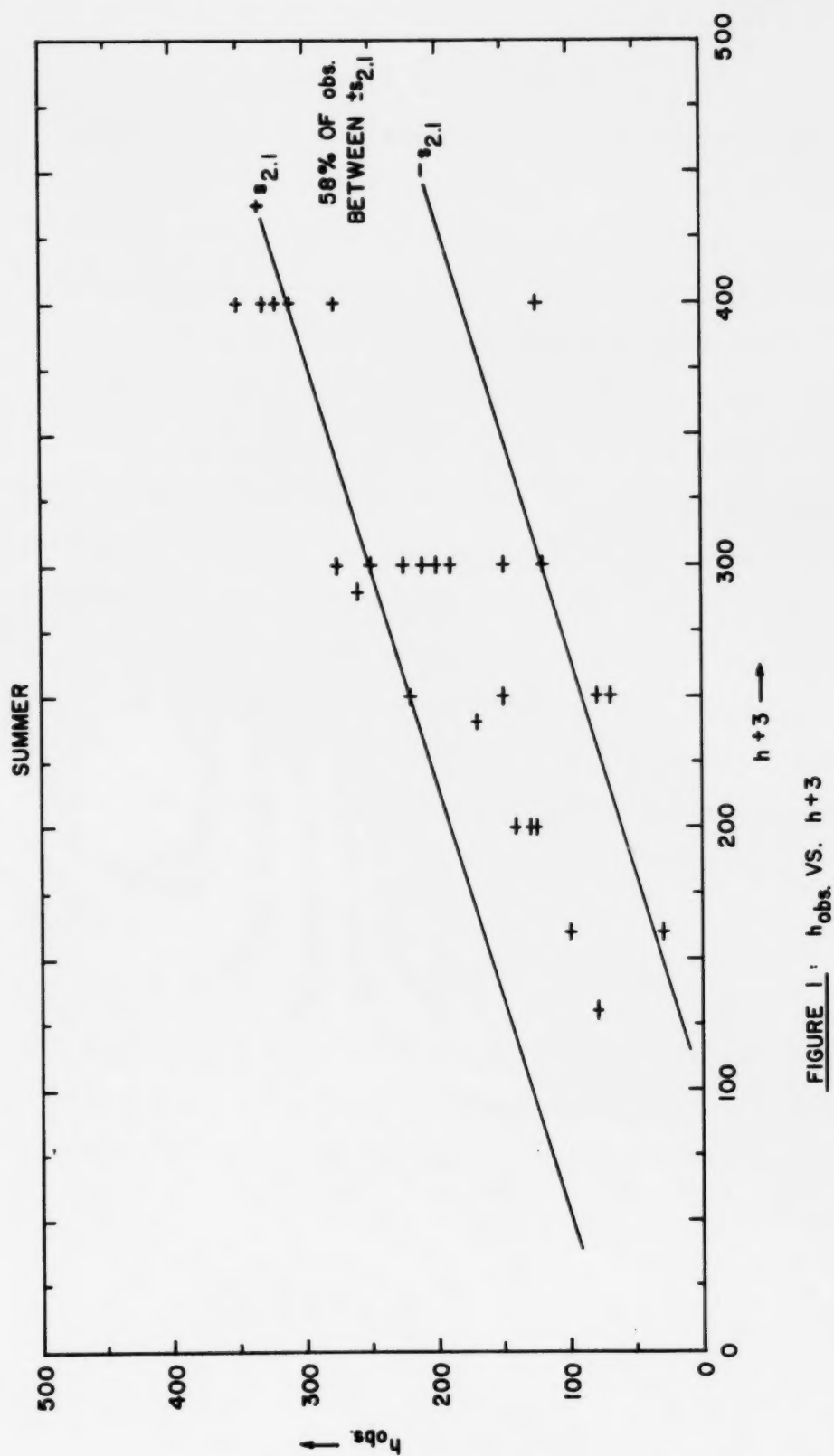


FIGURE 1: h_{obs} VS. $h+3$

VI OTHER CONTRIBUTIONS

Part 3

SO₂ CONCENTRATIONS AT KEYSTONE, PA.

R. Boomer

H. Panofsky

3.0 SO₂ CONCENTRATIONS AT KEYSTONE, PA.

R. Boomer and H. Panofsky, Research in Progress

3.1 The Purpose of the Project

For several years, SO₂ from the high stacks at the Keystone power plant near Indiana, Pennsylvania, was monitored along with the meteorological conditions.

The SO₂ concentrations were measured by helicopter through plume cross sections at various distances downstream of the plant and surface concentrations obtained from bubblers. This study primarily concerns the bubbler data.

Since dispersion and plume rise are controlled by wind and stability conditions, surface concentrations should be statistically related to the wind and temperature structure. In practice, wind at one level, and insolation, which are often available, could be used as surrogate predictors for the more complex wind and temperature information required.

It was therefore decided to statistically analyze the relation between surface concentration of SO₂, wind at one level, and insolation. Next, a simple technique was developed for estimating maximum ground concentration for a day for which wind and insolation could be obtained.

3.2 Analysis

The first step was to analyze the distribution of bubbler data for various dates. Isopleths of ground concentrations were constructed as function of time and distance from the stacks. Maximum concentrations generally occurred at 11 a.m. on sunny days.

Based on that information, the maximum concentration was determined separately for each day. These were plotted as functions of insolation and wind speed at the top of the stack. Fig. (1) shows the resulting isopleths. The greatest concentrations occurred on days when medium wind (~ 4 m/sec) and medium insolation. Presumably, on days with light winds, the effective stack height was too great for severe ground pollution; and for strong winds, the concentrations aloft were too small.

An attempt was made to account for the observed ground concentrations. First, vertical average concentrations were determined by summing the concentrations measured by helicopter in the center of the plume. It was expected that the vertically averaged concentrations would be an upper limit to the ground concentrations, which would exist right after fumigation. But there were many examples where the maximum ground concentrations exceeded the vertically averaged concentrations in the center of the plume.

This apparent discrepancy was probably caused by an inconsistency in time. The helicopter soundings were made early in the morning (~ 8 a.m.) but the maximum surface concentrations occurred, as mentioned, about 11 a.m. At 8 a.m. wind direction turned significantly with height, a factor that contributes to lateral spread. As Fig. (2) shows, the turning with height decreases to almost nothing at noon due to the decreased hydrostatic stability. Hence the width of the plume at 11 a.m. would be less than at 8 a.m. and central concentrations larger. Unfortunately, no helicopter soundings were made near 11 a.m.

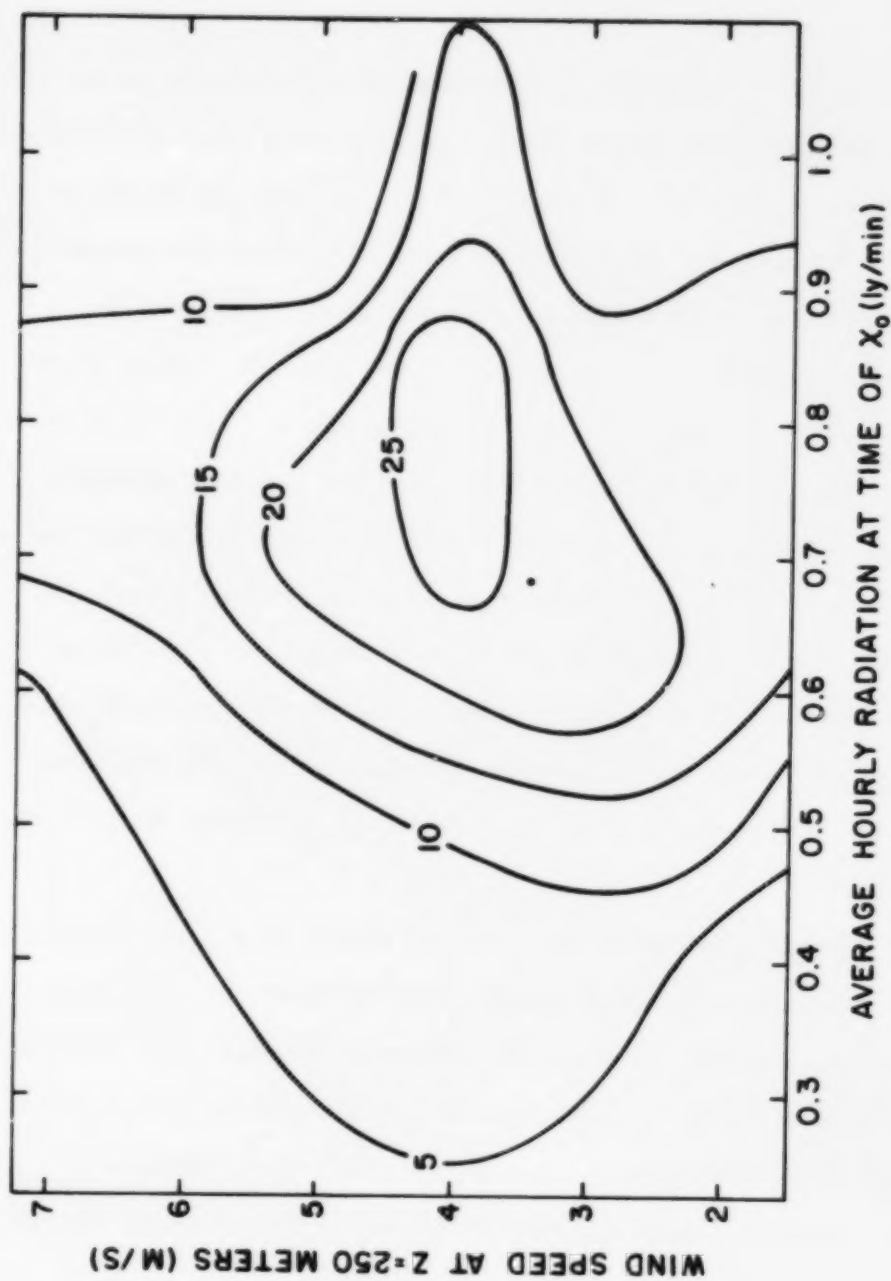


FIGURE 1 : CONCENTRATION ISOPLETHS AS A FUNCTION OF INSOLATION AND WINDSPEED.

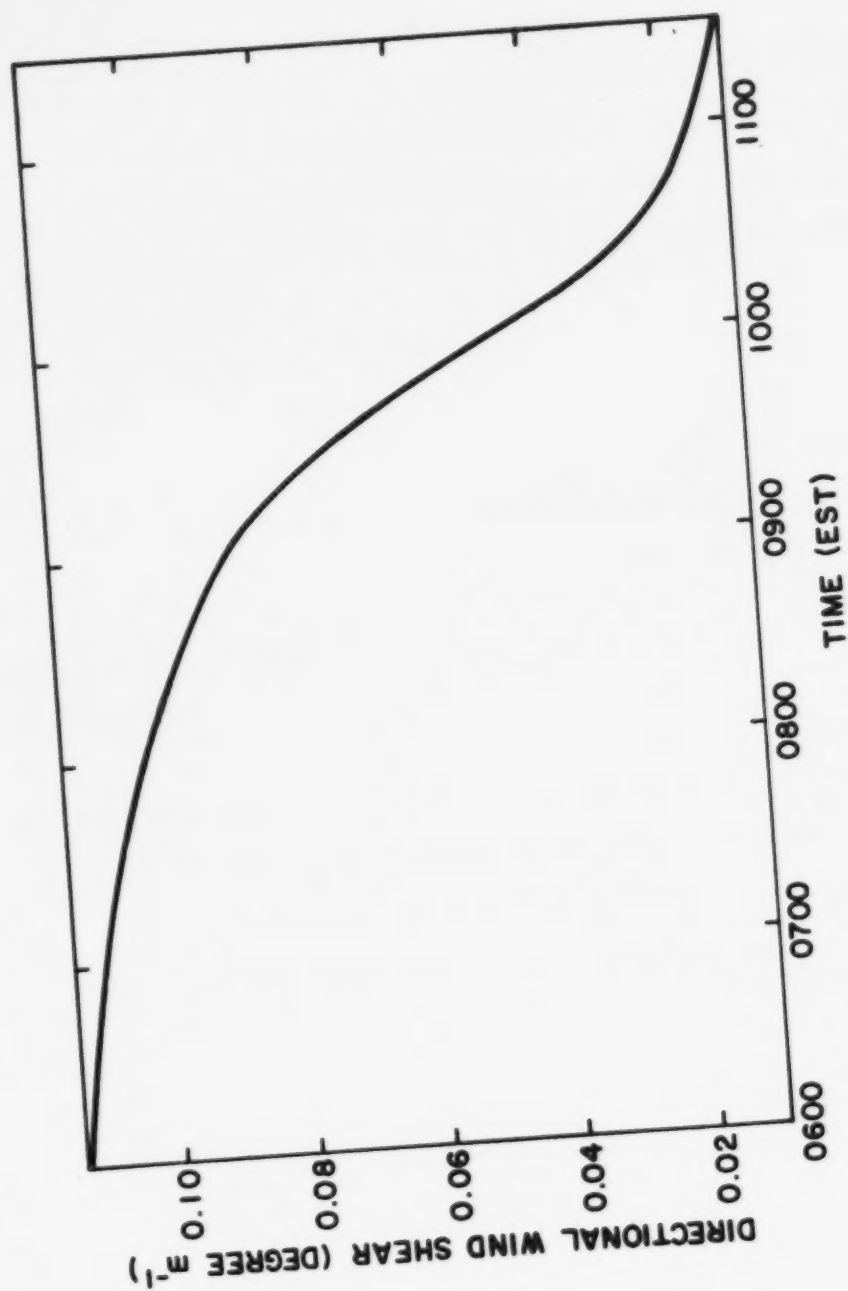


FIGURE 2. DIRECTIONAL WIND SHEAR AS A FUNCTION OF TIME.

A more direct attempt at accounting for the 11 a.m. concentration was based on estimates of σ_h (lateral standard deviation of mass) by Pasquill's method. Then, two alternate formulae were tried to estimate the concentration, one based on the assumption of vertically uniform distribution

$$\frac{2Q}{\sqrt{2\pi \bar{U} H \sigma_y}} \quad (1)$$

(where H is the height of the top of the plume) and the other on a completely Gaussian model

$$X_0 = \frac{Q}{\pi \bar{U} \sigma_y \sigma_z} \quad (2)$$

where σ_z was also found by Pasquill's method, $\bar{U}$ was the mean speed below H. In practice, Eq. (1) was almost never exceeded, and (2) was usually exceeded. Hence, we conclude that we cannot predict actual ground maximum concentrations, but only prescribe probable upper and lower limits.